

The term "protein tyrosine kinase," or PTK, refers to an enzyme that transfers the high energy phosphate of adenosine triphosphate to a tyrosine residue located on a protein target.

5 A protein tyrosine kinase catalytic domain of the invention can originate from receptor protein tyrosine kinases that bind fibroblast growth factor (FGF). These protein tyrosine kinases are known as "FGFR" herein, and can relate to one member of the FGFR family, such as  
10 FGFR1.

The term "catalytic domain" refers to the region of a protein that can exist as a separate entity from the protein. The catalytic domain of a protein tyrosine kinase is characterized as having considerable amino  
15 acid identity to the catalytic domain of other protein tyrosine kinases. Considerable amino acid identity preferably refers to at least 30% identity, more preferably at least 35% identity, and most preferably at least 40% identity. These degrees of amino acid  
20 identity refer to the identity between different protein tyrosine kinase families. Amino acid identity for members of a given protein tyrosine kinase family range from 55% to 90%. The catalytic domain may be functional as a separate entity. The catalytic domain of a protein  
25 tyrosine kinase is also characterized as a polypeptide that is soluble in solution.

The term "identity" identity as used herein refers to a property of sequences that measures their similarity or relationship. Identity is measured by  
30 dividing the number of identical residues in the two sequences by the total number of residues and

5 multiplying the product by 100. Thus, two copies of exactly the same sequence have 100% identity, but sequences that are less highly conserved and have deletions, additions, or replacements have a lower degree of identity. Those skilled in the art will recognize that several computer programs are available for determining sequence identity.

10 The term "functional" refers to the ability of a catalytic domain to convert a substrate into a product by phosphorylating the substrate. The term "functional" also relates to the ability of a catalytic domain to bind natural binding partners. The catalytic region may comprise an N-terminal tail, a catalytic core, and a C-terminal tail. The catalytic core is a polypeptide  
15 that can be functional in terms of catalysis. N- and C-terminal tails are polypeptide regions that may not confer appreciable functionality in terms of catalysis, but may confer functionality in terms of modulator specificity.

20 A polypeptide can exist as a catalytic domain eventhough it is not functional. For example, a polypeptide corresponding to a catalytic domain may not be functional if it does not harbor phosphate moieties in key areas. Multiple examples of phosphorylation-  
25 state dependent function are well documented in the art. Therefore, a catalytic domain can also exist without being functional. A measure of a protein kinase catalytic domain is a polypeptide that is homologous to other protein kinase catalytic domains.

30 The term "polypeptide" refers to an amino acid chain representing a portion of, or the entire sequence



of, amino acids comprising a protein.

A preferred embodiment of the invention includes a crystalline form of a PTK that is a receptor PTK.

Receptors are proteins that straddle the inside and  
5 outside of the cell membrane. Receptor PTKs comprise an extracellular region, a transmembrane region, and an intracellular region comprising a catalytic domain.

Another preferred embodiment of the invention is the crystalline form of a receptor PTK selected from the  
10 group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

Yet another preferred embodiment of the invention is the crystalline form of a PTK that is a non-receptor PTK. Non-receptor PTKs are located inside the cell and  
15 do not harbor extracellular or membrane-spanning polypeptides attached to the polypeptide corresponding to the catalytic domain. Non-receptor PTKs may harbor fatty acids or lipids, which can impart a membrane associated character to a PTK. In preferred embodiments  
20 of the invention, crystalline forms of non-receptor PTKs are selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In still another preferred embodiment, the invention features a crystalline form of a PTK that  
25 comprises a heavy metal atom. These types of crystals can be referred to as derivative crystals.

The term "derivative crystal" refers to a crystal where the polypeptide is in association with one or more heavy-metal atoms.

30 The term "association" refers to a condition of proximity between a chemical entity or compound, or

portions or fragments thereof, and tyrosine kinase domain protein, or portions or fragments thereof. The association may be non-covalent, i.e., where the juxtaposition is energetically favored by, e.g., hydrogen-bonding, van der Waals, electrostatic or hydrophobic interactions, or it may be covalent.

The term "heavy metal atom" refers to an atom that is a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

In a preferred embodiment, the invention features a crystal of an FGF receptor tyrosine kinase domain protein. The FGF receptor tyrosine kinase domain protein can relate to FGFR1.

The term "FGFR1" refers to one member of multiple receptor PTKs that are homologous to one another and bind FGF. In this context, the term "homologous" refers to at least 70% amino acid identity between two members of the FGFR family.

The term "FGFR1" can also refer to a mutant of human FGFR1 which is characterized by the amino acid sequence of SEQ ID NO:2. As compared to human FGFR1, FGFR1 contains the following amino acid substitutions: Cys-488 → Ala, Cys-584 → Ser, Leu-457 → Val, and has an additional five amino acid residues at the N-terminus (Ser-Ala-Ala-Gly-Thr).

The term "human FGFR1" refers to the tyrosine kinase domain of human fibroblast growth factor receptor 1 ("FGFR1") having the amino acid sequence of SEQ ID

NO:1. Generally, human FGFR1 comprises a 310 amino acid residue fragment (residues 456 to 765) of human FGFR1.

The term "mutant" refers to a polypeptide which is obtained by replacing at least one amino acid residue in a native tyrosine kinase domain with a different amino acid residue. Mutation can be accomplished by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native tyrosine kinase domain having substantially the same three-dimensional structure as the native tyrosine kinase domain from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the C $\alpha$  atoms of the native tyrosine kinase are included in the superposition. A mutant may have, but need not have, PTK activity.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 1.

The term "atomic structural coordinates" as used herein refers to a data set that defines the three dimensional structure of a molecule or molecules. Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the

resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed by a person of ordinary skill in the art as identical. Hence, the structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 are not limited to the values defined therein.

In other preferred embodiments, the invention features a crystalline form of the polypeptide in association with a compound. These types of crystalline forms can be referred to as co-crystals. The compound may be a cofactor, substrate, substrate analog, inhibitor, or allosteric effector.

The term "compound" refers to an organic molecule. The term "organic molecule" refers to a molecule which has at least one carbon atom in its structure. The compound can have a molecular weight of less than 6kDa. Both the geometry of the compound and the interactions formed between the compound and the polypeptide preferably govern high affinity binding between the two molecules. High affinity binding is preferably governed by a dissociation equilibrium constant on the order of  $10^{-6}$  M or less. The compound is preferably a modulator that alters the function of a PTK.

The term "function," in reference to the effect of a modulator on PTK function, refers to the ability of a modulator to enhance or inhibit the catalytic activity of a PTK.

The term "catalytic activity", in the context of the invention, defines the ability of a PTK to phosphorylate a substrate polypeptide. Catalytic

activity can be measured, for example, by determining the amount of a substrate converted to a product as a function of time. The conversion of the substrate to a product occurs at the active-site of the PTK.

5           The term "active-site" refers to a cavity located in the PTK in which one or more substrate molecules may bind. Addition of a modulator to cells expressing a PTK may enhance (activate) or lower (inhibit) the catalytic activity of the PTK.

10           A small number of inhibitors of PTK catalytic activity are known in the art. Small molecule inhibitors may modulate PTK function by blocking the binding of substrates. Indolinone compounds, for example, may bind to the active-site of PTK catalytic domains and inhibit them effectively, as measured by  
15           inhibition constants on the order of  $10^{-6}$  M or less.

          Activators of PTK intracellular regions can enhance PTK function by interacting with both the PTK catalytic domain and the substrate. Activators may also promote  
20           dimerization of PTKs and thus activate them by bringing them into close proximity with one another. In addition, activators may operate by promoting a conformational change in the intracellular region of the PTK such that the catalytic region modifies substrates  
25           at a faster rate in the presence of the activator.

          The term "function" can also refer to the ability of a modulator to enhance or inhibit the association between a PTK and a natural binding partner.

          The term "natural binding partner" refers to a  
30           polypeptide that normally binds to a PTK in a cell. These natural binding partners can play a role in

propagating a signal in a PTK signal transduction process. The natural binding partner can bind to a PTK with high affinity. High affinity represents an equilibrium binding constant on the order of  $10^{-6}$  M or less. However, a natural binding partner can also transiently interact with a PTK and chemically modify it. PTK natural binding partners are chosen from a group consisting of, but not limited to, src homology 2 (SH2) or 3 (SH3) domains, other phosphoryl tyrosine binding (PTB) domains, nucleotide exchange factors, and other protein kinases or protein phosphatases.

The term "interactions" refers to hydrophobic, aromatic, and ionic forces and hydrogen bonds formed between atoms in the modulator and the enzyme active-site.

The term "cofactor" refers to a compound that may, in addition to the substrate, bind to a protein and undergo a chemical reaction. Multiple co-factors are nucleotides or nucleotide derivatives, such as phosphate and nicotinamide derivatives of adenosine.

The term "substrate" refers to a compound that reacts with an enzyme. Enzymes can catalyze a specific reaction on a specific substrate. For example, PTKs can phosphorylate specific protein and peptide substrates on tyrosine moieties. In addition, nucleotides can act as substrates for protein kinases.

The term "substrate analog" refers to a compound that is structurally similar, but not identical, to a substrate. The substrate analog may be a nucleotide analog. Examples of nucleotide analogs are described below.

The term "inhibitor" refers to a compound that decreases the cellular function of a protein kinase. The protein kinase function is preferably the interaction with a natural binding partner and more preferably catalytic activity.

The term "allosteric effector" refers to a compound that causes allosteric interactions in a protein. The term "allosteric interactions" refers to interactions between separate sites on a protein. The sites can be different from the active site. The allosteric effector can enhance or inhibit catalytic activity by binding to a site that may be different than the active site.

The term "co-crystal" refers to a crystal where the polypeptide is in association with one or more compounds.

In preferred embodiments, a co-crystal of the invention can be in association with a heavy metal atom. Examples of heavy metal atoms are described above.

In other preferred embodiments, the invention features a co-crystal comprising the crystalline form of the polypeptide in association with a compound, where the compound is a non-hydrolyzable analog of ATP. These analogs can be referred to as nucleotide analogs.

The term "ATP" refers to the chemical compound adenosine triphosphate.

The term "non-hydrolyzable" refers to a compound having a covalent bond that does not readily react with water. Examples of non-hydrolyzable analogs of ATP are AMP-PNP and AMP-PCP, whose structures are well known to those skilled in the art.

The term "AMP-PNP" refers to adenylyl

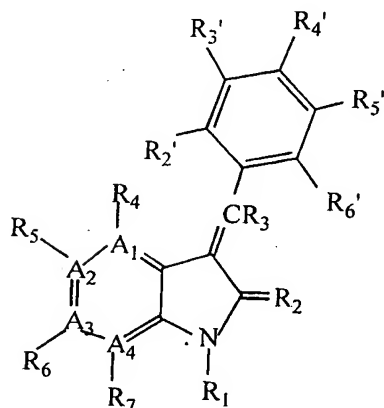
imidodiphosphate, a non-hydrolyzable analog of ATP.

The term "AMP-PCP" refers to adenylyl diphosphonate, a non-hydrolyzable analogue of ATP.

5 In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 2.

In preferred embodiments, the invention relates to crystalline forms, where the compound in association with the polypeptide is an indolinone.

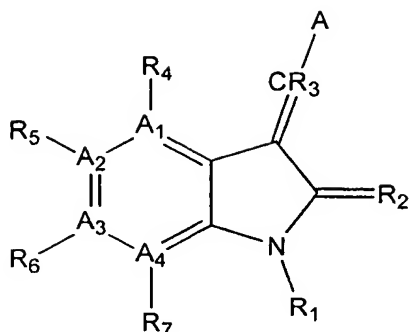
10 Certain indolinones are specific modulators of PTK function. A preferred embodiment of the invention is the crystalline form of a PTK complexed with an indolinone of formula I or II:



(I)



15



(II)

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, where:

- (a) A<sub>1</sub>, A<sub>2</sub>, A<sub>3</sub>, and A<sub>4</sub> are independently carbon or nitrogen;
- (b) R<sub>1</sub> is hydrogen or alkyl;
- (c) R<sub>2</sub> is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
- (d) R<sub>3</sub> is hydrogen;
- (e) R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> are optionally present, and are either (i) independently selected from the group consisting of alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR' or (ii) any two adjacent R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> taken together form a fused ring with the aryl portion of the indole-based portion of the indolinone;
- (f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R,

and CONRR';

(g) n is 0, 1, 2, or 3;

(h) R is hydrogen, alkyl or aryl;

(i) R' is hydrogen, alkyl or aryl; and

5 (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 10 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, 15 SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R or CONRR'.

The term "pharmaceutically acceptable salt" refers to those salts which retain the biological activity and 20 properties of the free bases. Pharmaceutically acceptable salts can be obtained by reaction with inorganic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid, methanesulfonic acid, ethanesulfonic acid, p-toluenesulfonic acid, salicylic acid and the like. 25

The term "prodrug" refers to an agent that is converted into the parent drug *in vivo*. Prodrugs may be easier to administer than the parent drug in some situations. For example, the prodrug may be 30 bioavailable by oral administration but the parent is not, or the prodrug may improve solubility to allow for

intravenous administration.

"Alkyl" refers to a straight-chain, branched or cyclic saturated aliphatic hydrocarbon. Preferably, the alkyl group has 1 to 12 carbons. More preferably, it is a lower alkyl of from 1 to 7 carbons, more preferably 1 to 4 carbons. Typical alkyl groups include methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tertiary butyl, pentyl, hexyl and the like. The alkyl group may be optionally substituted with one or more substituents are selected from the group consisting of hydroxyl, cyano, alkoxy, =O, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkenyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon group containing at least one carbon-carbon double bond. Preferably, the alkenyl group has 2 to 12 carbons. More preferably it is a lower alkenyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkenyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =O, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkynyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon containing at least one carbon-carbon triple bond. Preferably, the alkynyl group has 2 to 12 carbons. More preferably it is a lower alkynyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkynyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =O, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkoxy" refers to an "O-alkyl" group.

"Aryl" refers to an aromatic group which has at least one ring having a conjugated pi-electron system and includes carbocyclic aryl, heterocyclic aryl and biaryl groups. The aryl group may be optionally substituted with one or more substituents selected from the group consisting of halogen, trihalomethyl, hydroxyl, SH, OH, NO<sub>2</sub>, amine, thioether, cyano, alkoxy, alkyl, and amino.

"Alkaryl" refers to an alkyl that is covalently joined to an aryl group. Preferably, the alkyl is a lower alkyl.

"Carbocyclic aryl" refers to an aryl group wherein the ring atoms are carbon.

"Heterocyclic aryl" refers to an aryl group having from 1 to 3 heteroatoms as ring atoms, the remainder of the ring atoms being carbon. Heteroatoms include oxygen, sulfur, and nitrogen. Thus, heterocyclic aryl groups include furanyl, thienyl, pyridyl, pyrrolyl, N-lower alkyl pyrrolo, pyrimidyl, pyrazinyl, imidazolyl and the like.

"Amide" refers to -C(O)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Thioamide" refers to -C(S)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Amine" refers to a -N(R')R'' group, where R' and R'' are independently selected from the group consisting of alkyl, aryl, and alkylaryl.

"Thioether" refers to -S-R, where R is alkyl, aryl, or alkylaryl.

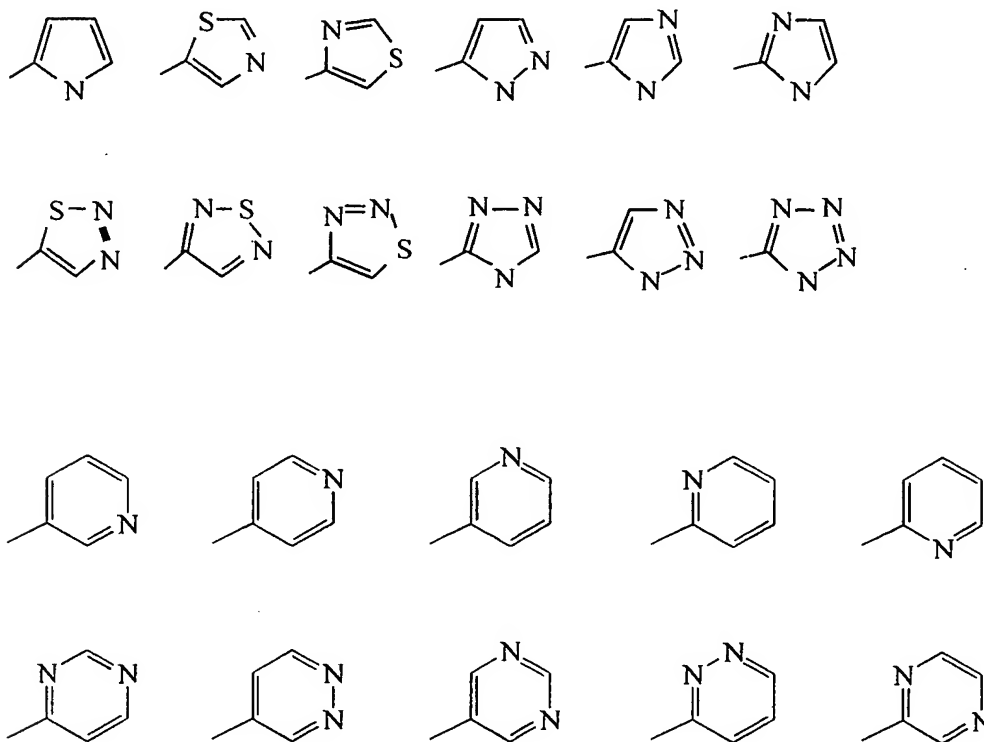
"Sulfonyl" refers to -S(O)<sub>2</sub>-R, where R is aryl, C(CN)=C-aryl, CH<sub>2</sub>CN, alkylaryl, sulfonamide, NH-alkyl, NH-

alkylaryl, or NH-aryl.

The term "acyl" denotes groups  $-C(O)R$ , where R is alkyl as defined above, such as formyl, acetyl, propionyl, or butyryl.

5 It is understood by those skilled in the art that when  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are nitrogen or sulfur that the corresponding  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$ , as well as the corresponding bond, do not exist.

10 Examples of indoles having such fused rings (as described in (e) (ii) above include the following:



15 The six membered rings shown above exemplify possible A rings in compound II.

Other preferred embodiments of the invention are crystalline forms comprising 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone as well as 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone. The polypeptide of these crystalline forms can be FGFR, and specifically, FGFR1.

In preferred embodiments, the crystalline forms of the invention can be defined by the structural coordinates set forth in Table 3 or Table 4.

The use of X-ray crystallography can elucidate the three dimensional structure of crystalline forms of the invention. The first characterization of crystalline forms by X-ray crystallography can determine the unit cell shape and its orientation in the crystal.

In other preferred embodiments, the invention features a crystal of an FGF receptor tyrosine kinase domain protein, where the crystal is characterized by having monoclinic unit cells. The crystal may also be characterized by having space group symmetry C2.

The term "unit cell" refers to the smallest and simplest volume element (i.e., parallelepiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The dimensions of the unit cell are defined by six numbers: dimensions a, b and c and angles  $\alpha$ ,  $\beta$  and  $\gamma$ . A crystal can be viewed as an efficiently packed array of multiple unit cells. Detailed descriptions of crystallographic terms are described in, which is hereby incorporated herein by reference in its entirety, including any drawings, figures, and tables.

The term "monoclinic unit cell" refers to a unit

cell where  $a \neq b \neq c$ ;  $\alpha = \gamma = 90^\circ$ ; and  $\beta > 90^\circ$ .

The term "space group" refers to the symmetry of a unit cell. In a space group designation (e.g., C2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance.

The term "lattice" in reference to crystal structures refers to the array of points defined by the vertices of packed unit cells.

The term "symmetry operations" refers to geometrically defined ways of exchanging equivalent parts of a unit cell, or exchanging equivalent molecules between two different unit cells. Examples of symmetry operations are screw axes, centers of inversion, and mirror planes.

In a preferred embodiment, the invention features a crystalline form, where the monoclinic unit cells have dimensions of about  $a=208.3 \text{ \AA}$ ,  $b=57.8 \text{ \AA}$ ,  $c=65.5 \text{ \AA}$  and  $\beta=107.2^\circ$ .

In a preferred embodiment, the invention features a FGFR1 crystal, where the monoclinic unit cells have dimensions of about  $a=211.6 \text{ \AA}$ ,  $b=51.3 \text{ \AA}$ ,  $c=66.1 \text{ \AA}$  and  $\beta=107.7^\circ$ .

In another aspect the invention features a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal

boundary of the catalytic domain.

The polypeptides of the invention can be isolated, enriched or purified. In addition, the crystalline forms of the invention can be formed from polypeptides that are isolated, enriched, or purified.

By "isolated" in reference to a polypeptide is meant a polymer of 6, 12, 18 or more amino acids conjugated to each other, including polypeptides that are isolated from a natural source or that are synthesized. The isolated polypeptides of the present invention are unique in the sense that they are not found in a pure or separated state in nature. Use of the term "isolated" indicates that a naturally occurring sequence has been removed from its normal cellular environment. Thus, the sequence may be in a cell-free solution or placed in a different cellular environment. The term does not imply that the sequence is the only amino acid chain present, but that it is essentially free (about 90 - 95% pure at least) of material naturally associated with it.

By the use of the term "enriched" in reference to a polypeptide it is meant that the specific amino acid sequence constitutes a significantly higher fraction (2 - 5 fold) of the total of amino acids present in the cells or solution of interest than in normal or diseased cells or in the cells from which the sequence was taken. This could be caused by a person by preferential reduction in the amount of other amino acids present, or by a preferential increase in the amount of the specific amino acid sequence of interest, or by a combination of the two. However, it should be noted that "enriched"



does not imply that there are no other amino acid sequences present, just that the relative amount of the sequence of interest has been significantly increased. The term significant here is used to indicate that the level of increase is useful to the person making such an increase, and generally means an increase relative to other amino acids of about at least 2 fold, more preferably at least 5 to 10 fold or even more. The term also does not imply that there are no amino acids from other sources. The other source amino acids may, for example, comprise amino acids encoded by a yeast or bacterial genome, or a cloning vector such as pUC19. The term is meant to cover only those situations in which a person has intervened to elevate the proportion of the desired nucleic acid.

It is also advantageous for some purposes that an amino acid sequence be in purified form. The term "purified" in reference to a polypeptide does not require absolute purity (such as a homogeneous preparation); instead, it represents an indication that the sequence is relatively purer than in the natural environment (compared to the natural level this level should be at least 2-5 fold greater, e.g., in terms of mg/ml). Purification of at least one order of magnitude, preferably two or three orders, and more preferably four or five orders of magnitude is expressly contemplated. The substance is preferably free of contamination at a functionally significant level, for example 90%, 95%, or 99% pure.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a

receptor PTK. The receptor PTK may have a three-dimensional structure substantially similar to that of the insulin receptor, even though the amino acid content may be different.

5 In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, where the non-insulin receptor tyrosine kinase is a cytoplasmic tyrosine kinase.

10 In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a receptor PTK, selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, or MUSK.

15 In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, or ACK.

20 In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a PTK, having the amino acid sequence shown in Table 1 or Table 2.

In another aspect, the invention features a method for creating crystalline forms described herein. The method may utilize the polypeptides described herein to form a crystal. The method comprises the steps of:

25 (a) mixing a volume of polypeptide solution with a reservoir solution; and

(b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container, under conditions suitable for crystallization.

30 These processes are described in detail in the

section entitled "Detailed Description of the Invention."

In another aspect, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps  
5 of: (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, where the polypeptide solution comprises 1 mg/mL to 60 mg/mL FGF-type tyrosine kinase domain protein, 10 mM to 200 mM  
10 buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and where the reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering  
15 agent and has a pH of about 5.5 to about 7.5; and (b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25°C until crystals form.

In a preferred embodiment, the invention features a  
20 method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of  
25 about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

30 In another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine

kinase domain polypeptide in crystalline form, where the polypeptide solution includes a compound such as a cofactor, substrate, substrate analog, inhibitor or allosteric effector.

5 In still another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the compound is a nucleotide analog, such as a non-hydrolyzable analog of ATP, or an indolinone.  
10 Indolinone compounds have the general structural formula as described herein.

In another aspect, the invention features a cDNA encoding an FGF receptor tyrosine kinase domain protein, where a coding strand of the cDNA has the nucleotide  
15 sequence of SEQ ID NO:5.

Another aspect of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by utilizing the structural  
20 coordinates of Table 1, Table 2, Table 3, and Table 4. These methods can relate to homology modeling, molecular replacement, and nuclear magnetic resonance methods.

In a preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structures by utilizing the  
25 coordinates of Table 1, Table 2, Table 3, or Table 4 in conjunction with the amino acid sequences of PTKs. This method of homology modeling comprises the steps of: (a) aligning the computer representation of an amino acid sequence of a PTK with unknown structure with that of a  
30 PTK with known structure, where alignment is achieved by matching homologous regions of the amino acid sequences;

(b) transferring the computer representation of an amino acid structure in the PTK sequence of known structure to a computer representation of a structure of the corresponding amino acid in the PTK sequence with  
5 unknown structure; and (c) determining low energy conformations of the resulting PTK structure.

The term "amino acid sequence" describes the order of amino acids in the amino acid chain comprising a polypeptide corresponding to the catalytic domain of a  
10 PTK.

The term "aligning" describes matching the beginning and the end of two or more amino acid sequences. Homologous amino acid sequences are placed on top of one another during the alignment process.

15 The term "homologous" describes amino acids in two sequences that are identical or have similar side-chain chemical groups (e.g., aliphatic, aromatic, polar, negatively charged, or positively charged).

The term "corresponding" refers to an amino acid  
20 that is aligned with another in the sequence alignment mentioned above.

The term "determining the low energy conformation" describes a process of changing the conformation of the PTK structure such that the structure is of low free  
25 energy. The PTK structure may or may not have molecules, such as modulators bound to it.

The term "low free energy" describes a state where the molecules are in a stable state as measured by the process. A stable state is achieved when favorable  
30 interactions are formed within the complex.

The term "favorable interactions" refers to

hydrophobic, aromatic, and ionic forces, and hydrogen bonds.

Another preferred embodiment of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure. This method is accomplished by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to an incomplete X-ray crystallographic data set for a PTK. The method comprises the steps of: (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals, where one data set is complete and the other is incomplete; and (b) determining a low energy conformation of the resulting PTK structure.

The term "incomplete data set" relates to a X-ray crystallographic data set that does not have enough information to give rise to a three dimensional structure.

In another preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to nuclear magnetic resonance (NMR) data of a PTK. This method comprises the steps of: (a) determining the secondary structure of a PTK structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The PTK structure may not be complexed with compounds or modulators.

The term "secondary structure" describes the arrangement of amino acids in a three dimensional

structure, such as in  $\alpha$ -helix or  $\beta$ -sheet elements.

The term "through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence.

The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

In another aspect, the invention features a method of identifying potential modulators of PTK function. These modulators are identified by docking a computer representation of a structure of a compound with a computer representation of a cavity formed by the active-site of a PTK. The computer representation of the PTK active-site structure can be defined by structural coordinates.

The term "chemical group" refers to moieties that can form hydrogen bonds, hydrophobic, aromatic, or ionic interactions.

The term "docking" refers to a process of placing a compound in close proximity with a PTK. The term can also refer to a process of finding low energy conformations of the compound/PTK complex.

A preferred embodiment of the invention is a method of identifying potential modulators of PTK function. The method involves utilizing the structural coordinates or a PTK three dimensional structure. The structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 can be utilized. The method comprises the steps of: (a) removing a computer representation of a PTK

structure and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the PTK; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying compounds that best fit the PTK active-site as potential modulators of PTK function. The initial PTK structure may or may not have compounds bound to it.

The term "favorable geometric fit" refers to a conformation of the compound-PTK complex where the surface area of the compound is in close proximity with the surface area of the active-site without forming unfavorable interactions. Unfavorable interactions can be steric hindrances between atoms in the compound and atoms in the PTK active-site.

The term "favorable complementary interactions" relates to hydrophobic, aromatic, ionic, and hydrogen bond donating, and hydrogen bond accepting forces formed between the compound and the PTK active-site.

The term "potential" qualifies the term "modulator of PTK function" because the potential modulator or PTK function has not yet been tested for activity *in vitro* or *in vivo*.

The term "best fit" describes compounds that complexed the most surface area in the complex and/or form the most favorable complementary interactions with the PTK in the screen in a given experiment.

Another preferred embodiment of the invention is a method of identifying potential modulators of PTK function. The method involves utilizing a three



dimensional structure of a PTK, with or without compounds bound to it. The method comprises the steps of: (a) modifying a computer representation of a PTK having one or more compounds bound to it, where the  
5 computer representations of the compound or compounds and PTK are defined by structural coordinates; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying the compounds that  
10 best fit the PTK active-site as potential modulators of PTK function.

The term "modifying" relates to deleting a chemical group or groups or adding a chemical group or groups. Computer representations of the chemical groups can be  
15 selected from a computer data base.

Yet another preferred embodiment of the invention is a method of identifying potential modulators of PTK function by operating modulator construction or modulator searching computer programs on the compounds  
20 complexed with the PTK. The method comprises the steps of: (a) removing a computer representation of one or more compounds complexed with a PTK; and (b) searching a data base for compounds similar to the removed compounds using a compound searching computer program, or  
25 replacing portions of the compounds complexed with the PTK with similar chemical structures from a data base using a compound construction computer program, where the representations of the compounds are defined by structural coordinates.

30 The term "operating" as used herein refers to utilizing the three-dimensional conformation of

molecules defined by the processes described herein in various computer programs.

The term "similar compound" refers to a compound in a computer data base that has a similar geometric structure as compounds that can bind to a PTK. The similar compound can also have similar chemical groups as the compounds that are either bound to the PTK or once bound to the PTK. The similar chemical groups can form complementary interactions with the PTK.

The term "compound searching computer program" describes a computer program that searches computer representations of compounds from a computer data base that have similar three dimensional structures and similar chemical groups as a compound of interest. The compound of interest is preferably an indolinone compound.

The term "similar chemical structures" refers to chemical groups that share similar geometry as portions of the compounds in complex with the PTK or compounds removed from the PTK structure. Similar chemical structures can also refer to chemical groups that may form similar complementary interactions as portions of the compounds in complex with the PTK or compounds removed from the PTK structure.

The term "replacing structures" refers to removing a portion of the compounds in complex with the PTK or compounds removed from the PTK structure and connecting the broken bonds to a similar chemical structure.

The term "compound construction computer program" describes a computer program that replaces computer representations of chemical groups in a compound with

groups from a computer data base. The compound is preferably an indolinone compound.

The term "similar three dimensional structure" describes two molecules with nearly identical shape and  
5 volume.

In another preferred embodiment of the invention, the PTK structures used in the modulator design or identification method of the invention are defined by the structural coordinates of Table 1, Table 2, Table 3,  
10 or Table 4.

The methods for using the crystalline forms and three dimensional structures of the invention can relate to a broad range of protein kinases. Thus, in preferred embodiments, the invention relates to a receptor PTK.  
15 The receptor PTK can be selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. The PTK may also exist as a non-receptor PTK. The non-receptor PTK can be selected from the group consisting  
20 of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In another aspect, the invention features a potential modulator of PTK function identified by methods disclosed in the invention.

25 A preferred embodiment of the invention is that the potential modulator of PTK function is an oxindolinone or a thiolindolinone of formula I or II disclosed above.

Another aspect of the invention is a method for synthesizing a potential modulator of PTK function or  
30 its pharmaceutically acceptable salts, isomers, metabolites, esters, amides, or prodrugs by a standard

synthetic method known in the art. Synthetic procedures are discussed below.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of PTK phosphorylation between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in the level of PTK phosphorylation.

The term "cells" refers to any type of cells either primary or cultured. Primary cells can be extracted directly from an organism while cultured cells rapidly divide and can be cultured in many successive rounds. Cells can be grown in a variety of containers including, but not limited to flasks, dishes, and well plates.

The term "administer" refers to a method of delivering a compound to cells. The compound can be prepared using a carrier such as dimethyl sulfoxide (DMSO) in an aqueous solution. The aqueous solution comprising the compound, also termed an "aqueous preparation", can be simply mixed into the medium bathing the layer of cells or microinjected into the cells themselves. The compounds may be administered to the cells using a suitable buffered solution.

The term "suitable buffered solution" refers to an aqueous preparation of the compound that comprises a salt that can control the pH of the solution at low concentrations. Because the salt exists at low

concentrations, the salt preferably does not alter the function of the cells.

The term "PTK phosphorylation" refers to the presence of phosphate on the PTK. Phosphates on PTKs  
5 can be identified by antibodies that bind them specifically with high affinity.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the  
10 steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of cell growth between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator  
15 as a modulator of PTK function based on the difference in cell growth.

The term "cell growth" refers to the rate at which a group of cells divides. Cell division rates can be readily measured by methods utilized by those skilled in  
20 the art.

Another aspect of the invention features a method of diagnosing a disease by identifying cells harboring a PTK with inappropriate activity. The method comprises the steps of: (a) administering a modulator of PTK  
25 function to cells; (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and (c) diagnosing a disease by characterizing cells harboring a PTK with inappropriate activity from the effect of the modulator  
30 on the difference in the rate of cell growth. The modulator can be identified by the methods of the

invention.

The term "inappropriate activity" refers to a PTK that regulates a step in a signal transduction process at a higher or lower rate than normal cells.

5 Aberrations in the rate of signal transduction can be caused by alterations in the stimulation of a receptor PTK by a growth factor, alterations in the activity of PTK-specific phosphatase, over-expression of a PTK in a cell, or mutations in the catalytic region of the PTK  
10 itself.

The term "signal transduction process" describes the steps in a cascade of events where an extracellular signal is transmitted into an intracellular signal.

15 The term "PTK-specific phosphatase" describes an enzyme that dephosphorylates a particular PTK and thereby regulates that PTK's activity.

Another aspect of the invention is a method of treating a disease associated with a PTK with inappropriate activity in a cellular organism, where the  
20 method comprises the steps of: (a) administering the modulator of PTK function to the organism, where the modulator is in an acceptable pharmaceutical preparation; and (b) activating or inhibiting the PTK function to treat the disease.

25 The term "organism" relates to any living being comprised of at least one cell. An organism can be as simple as one eukaryotic cell or as complex as a mammal.

The term "administering", in reference to an organism, refers to a method of introducing the compound  
30 to the organism. The compound can be administered when the cells or tissues of the organism exist within the

organism or outside of the organism. Cells existing outside the organism can be maintained or grown in cell culture dishes. For cells harbored within the organism, many techniques exist in the art to administer  
5 compounds, including (but not limited to) oral, parenteral, dermal, and injection applications. For cells outside of the patient, multiple techniques exist in the art to administer the compounds, including (but not limited to) cell microinjection techniques,  
10 transformation techniques, and carrier techniques.

The term "pharmaceutically acceptable composition" refers to a preparation comprising the modulator of PTK activity. The composition is acceptable if it does not appreciably cause irritations to the organism  
15 administered the compound.

Preferred embodiments of the of the invention are that the PTK is a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK-1, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.  
20 Other preferred embodiments of the invention are that the PTK is a non-receptor PTK selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

The summary of the invention described above is non-limiting and other features and advantages of the  
25 invention will be apparent from the following detailed description, and from the claims.

#### BRIEF DESCRIPTION OF THE FIGURES

30 FIG. 1 provides a ribbon diagram of the structure of FGFR1 showing the side chains of tyrosines Tyr-653

and Tyr-654 and the  $\alpha$  helical ( $\alpha$ C,  $\alpha$ D,  $\alpha$ E,  $\alpha$ EF,  $\alpha$ F- $\alpha$ I),  $\beta$  strand ( $\beta$ 1- $\beta$ 5,  $\beta$ 7,  $\beta$ 8), nucleotide-binding loop, catalytic loop, activation loop and kinase insert regions of the molecule. The termini are denoted by N and C. The loop between  $\beta$ 2 and  $\beta$ 3 is disordered, indicated by a break in the chain in this region.

FIG. 2 provides a stereo view of a  $C_{\alpha}$  trace of FGFR1 shown in the same orientation as FIG. 1, with every tenth amino acid residue marked with a filled circle and every twentieth amino acid residue labeled with a residue number.

FIG. 3 provides a structure-based sequence alignment of human fibroblast growth factor receptor 1 (FGFR1), human fibroblast growth factor receptor 2 (FGFR2), human fibroblast growth factor receptor 3 (FGFR3), human fibroblast growth factor receptor 4 (FGFR4), a *D. melanogaster* homolog (DFGFR1), a *C. elegans* homolog (EGL-15) and insulin receptor tyrosine kinase (IRK).

FIGS. 4A and 4B provide ribbon diagrams of the N-terminal lobes (4A) and C-terminal lobes (4B) of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\beta$  sheets (4A) or  $\alpha$ -helices (4B) of the two proteins have been superimposed.

FIG. 5 illustrates the side-chain positions of the tyrosine autophosphorylation sites of FGFR1 on the backbone representation of FGFR1.

FIGS. 6A and 6B are amino acid sequence alignments of the catalytic domains of PTKs, including receptor and non-receptor type PTKs. FIG. 6A depicts one representative member from each of the eighteen subfamilies of receptor tyrosine kinases. FIG. 6B



depicts one representative member from each of the subfamilies of cytoplasmic tyrosine kinases. In FIGS. 6A and 6B highly conserved residues are boxed. The position of the glycine-rich domain, kinase insert, catalytic loop, and activation loop are indicated. The numbering is for human FGF-receptor.

BRIEF DESCRIPTION OF THE CRYSTALLOGRAPHIC ATOMIC  
STRUCTURAL COORDINATES

The crystallographic structural coordinates are located at the end of the section entitled "Examples" and before the claims. Three sets of coordinates can be found in the Protein Data Bank under accession names 1FGK, 1AGW, and 1FGI. The 1FGK coordinates correspond to those listed in Table 1, the 1AGW coordinates correspond to those listed in Table 4, and the 1FGI coordinates correspond to those listed in Table 3. The 1AGW and 1FGI coordinate sets will be publically available in March 1998.

Table 1 provides the atomic structure coordinates of native FGFR1 crystals of the invention as determined by X-ray crystallography; and

Table 2 provides the atomic structure coordinates of FGFR1:AMP-PCP co-crystals of the invention as determined by X-ray crystallography.

Table 3 lists crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The columns (from left to right) are descriptions of the atoms by number and type, amino acid and number containing the atom, the x coordinate, y

coordinate, z coordinate, bond connectivity, and temperature factor. All of these parameters are well defined in the art.

Table 4 is a file of crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[4-(4-formylpiperazine-1-yl)benzylidenyl]-2-indolinone. The columns are as described in Table 3.

#### DETAILED DESCRIPTION OF THE INVENTION

The present invention is directed to the design and identification of modulators of protein tyrosine kinase function that are PTK subfamily specific, non-hydrolyzable under acidic conditions, and highly bioavailable. The three dimensional structures of a PTK optionally complexed with compounds can facilitate design and identification of modulators of PTK function.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes. Schlessinger and Ullrich, 1992, *Neuron* 9: 383-391. The PTK family is subdivided into members that are receptors and those that are non-receptors. The PTK receptor family contains multiple subfamilies, one of which is the fibroblast growth factor receptor (FGF-R) PTK which is a molecule implicated in regulating angiogenesis as well as cellular proliferation and differentiation. Givol and Yayon, 1992, *FASEB J.* 6 (15): 3362-3369.

FGF-R1 can mediate cellular functions by its role in one or more cellular signal transduction processes. Cellular signal transduction processes comprise multiple steps that convert an extracellular signal into an

intracellular signal.

Receptor PTK mediated signal transduction is initiated by binding a specific extracellular ligand, followed by receptor dimerization, and subsequent autophosphorylation of the receptor PTK. The phosphate groups are binding sites for intracellular signal transduction molecules which leads to the formation of protein complexes at the cell membrane. These complexes facilitate an appropriate cellular effect (e.g., cell division, metabolic effects to the extracellular microenvironment) in response to the ligand that began the cascade of events.

Receptor PTKs function as binding sites for several intracellular proteins. Intracellular PTK binding proteins are divided into two principal groups: (1) those which harbor a catalytic domain; and (2) those which lack such a domain but serve as adapters and associate with catalytically active molecules. Songyang et al., 1993, *Cell* 72:767-778. SH2 (src homology) domains are common adaptors found in proteins which directly bind to the receptor PTK. SH2 domains are harbored by PTK binding proteins of both groups mentioned above. Fantl et al., 1992, *Cell* 69:413-423; Songyang et al., 1994, *Mol. Cell. Biol.* 14:2777-2785; Songyang et al., 1993, *Cell* 72:767-778; and Koch et al., 1991, *Science* 252:668-678.

The specificity of the interactions between receptor PTKs and the SH2 domains of their binding proteins is determined by the amino acid residues immediately surrounding the phosphorylated tyrosine residue. Differences in the binding affinities of SH2

domains is correlated with the observed differences in substrate phosphorylation profiles of downstream molecules in the signal transduction process. Songyang et al., 1993, *Cell* 72:767-778. These observations suggest that the function of each receptor PTK is determined not only by its pattern of expression and ligand availability but also by the array of downstream signal transduction pathways that are activated by a particular receptor. Thus, PTKs provide a controlling regulatory role in signal transduction processes as a consequence of autophosphorylation.

PTK-mediated signal transduction regulates cell proliferative, differentiation, and metabolic responses in cells. Therefore, inappropriate PTK activity can result in a wide array of disorders and diseases. These disorders, which are described below, may be treated by the modulators of PTK function designed or identified by the methods disclosed herein.

The present invention also relates to crystalline polypeptides corresponding to the catalytic domain of receptor tyrosine kinases. Such tyrosine kinases include receptors of a class that are not covalently cross-linked but are understood to undergo ligand-induced dimerization, as well as cytoplasmic tyrosine kinases. Preferably, the crystalline catalytic domains are of sufficient quality to allow for the determination of a three-dimensional X-ray diffraction structure to a resolution of about 1.5 Å to about 2.5 Å. The invention also relates to methods for preparing and crystallizing the polypeptides. The polypeptides themselves, as well as information derived from their crystal structures can

be used to analyze and modify tyrosine kinase activity as well as to identify compounds that interact with the catalytic domain.

The polypeptides of the invention are designed on the basis of the structure of a region in the cytoplasmic domain of the receptor tyrosine kinase that contains the catalytic domain. By way of illustration, FIG. 6A shows the amino acid sequence alignment of the catalytic domains of eighteen human receptor tyrosine kinases; one representative member from each of the eighteen subfamilies is shown. FIG. 6B shows the alignment for cytoplasmic kinases. The applicants have discovered and determined the boundaries of the domain required for crystallization of the resulting polypeptide. Surprisingly, these boundaries differ from that required for catalytic activity. For example, referring to FIG. 6A, the domain required for catalytic activity is generally believed to span about 7 amino acid residues upstream of the first glycine (FIG. 6A residue number 485) of the N-terminal glycine-rich region through about 10 residues beyond the C-terminal conserved arginine (FIG. 6A, residue number 744). However, the additional sequence upstream of the N-terminal glycine-rich region and downstream of the C-terminal conserved arginine can be required for crystallization. In particular, at least about 20 amino acid residues (+/- 5 amino acid residues) upstream of the first glycine (i.e., FIG. 6A, residue number 485) in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues (+/- 5 amino acid residues) downstream of the conserved

arginine (i.e., FIG. 6A, residue number 744) located at the C-terminal boundary of the catalytic domain can be required to engineer a polypeptide suitable for crystallization.

5 In those situations where the resulting polypeptide contains cysteine residues that interfere with crystallization (e.g., cysteine residue numbers 488 and 584 in the FGF-R1 sequence shown in FIG. 6A), such cysteine residues can be substituted with an appropriate  
10 amino acid that does not readily form covalent bonds with other amino acid residues under crystallization conditions; e.g., by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non- $\beta$ -stranded segment, based on secondary structure  
15 assignments, are good candidates for replacement. For example, cysteines located in regions corresponding to the glycine-rich-loop, the kinase insert, the juxtamembrane region or the activation loop are prime candidates for replacement. However, substitutions of  
20 cysteine residues that are conserved among the kinases (e.g., FIG. 6A at positions 725 and 736) are preferably avoided.

#### I. PTK Associated Diseases

25 Blood vessel proliferative disorders refer to angiogenic and vasculogenic disorders generally resulting in abnormal proliferation of blood vessels. The formation and spreading of blood vessels play  
30 important roles in a variety of physiological processes such as embryonic development, corpus luteum formation, wound healing and organ regeneration. They also play a

pivotal role in cancer development. Other examples of blood vessel proliferation disorders include arthritis, where new capillary blood vessels invade the joint and destroy cartilage, and ocular diseases, like diabetic retinopathy, where new capillaries in the retina invade the vitreous, bleed and cause blindness. Conversely, disorders related to the shrinkage, contraction or closing of blood vessels are implicated in such diseases as restenosis.

10           Fibrotic disorders refer to the abnormal formation of extracellular matrix. Examples of fibrotic disorders include hepatic cirrhosis and mesangial cell proliferative disorders. Hepatic cirrhosis is characterized by the increase in extracellular matrix constituents resulting in the formation of a hepatic scar. Hepatic cirrhosis can cause diseases such as cirrhosis of the liver. An increased extracellular matrix resulting in a hepatic scar can also be caused by viral infection such as hepatitis.

20           Mesangial cell proliferative disorders refer to disorders brought about by abnormal proliferation of mesangial cells. Mesangial proliferative disorders include various human renal diseases, such as glomerulonephritis, diabetic nephropathy, malignant nephrosclerosis, thrombotic microangiopathy syndromes, transplant rejection, and glomerulopathies. The PDGF-R has been implicated in the maintenance of mesangial cell proliferation. Floege et al., 1993, *Kidney International* 43:47S-54S.

30           PTKs are directly associated with the cell proliferative disorders described above. For example,

some members of the receptor PTK family have been associated with the development of cancer. Some of these receptors, like EGFR (Tuzi et al., 1991, *Br. J. Cancer* 63:227-233; Torp et al., 1992, *APMIS* 100:713-719) HER2/neu (Slamon et al., 1989, *Science* 244:707-712) and PDGF-R (Kumabe et al., 1992, *Oncogene* 7:627-633) are over-expressed in many tumors and/or persistently activated by autocrine loops. In fact, PTK over-expression (Akbasak and Suner-Akbasak et al., 1992, *J. Neurol. Sci.* 111:119-133; Dickson et al., 1992, *Cancer Treatment Res.* 61:249-273; Korc et al., 1992, *J. Clin. Invest.* 90:1352-1360) and autocrine loop stimulation (Lee and Donoghue, 1992, *J. Cell. Biol.* 118:1057-1070; Korc et al., *supra*; Akbasak and Suner-Akbasak et al., *supra*) account for the most common and severe cancers. For example, EGFR is associated with squamous cell carcinoma, astrocytoma, glioblastoma, head and neck cancer, lung cancer and bladder cancer. HER2 is associated with breast, ovarian, gastric, lung, pancreas and bladder cancer. PDGF-R is associated with glioblastoma, lung, ovarian, melanoma and prostate cancer. The receptor PTK c-met is generally associated with hepatocarcinogenesis and thus hepatocellular carcinoma. Additionally, c-met is linked to malignant tumor formation. More specifically, c-met has been associated with, among other cancers, colorectal, thyroid, pancreatic and gastric carcinoma, leukemia and lymphoma. Additionally, over-expression of the c-met gene has been detected in patients with Hodgkins disease, Burkitts disease, and the lymphoma cell line. The IGF-I receptor PTK, in addition to being



implicated in nutritional support and in type-II diabetes, is also associated with several types of cancers. For example, IGF-I has been implicated as an autocrine growth stimulator for several tumor types, e.g. human breast cancer carcinoma cells (Arteaga et al., 1989, *J. Clin. Invest.* 84:1418-1423) and small lung tumor cells (Macauley et al., 1990, *Cancer Res.* 50:2511-2517). In addition, IGF-I, integrally involved in the normal growth and differentiation of the nervous system, appears to be an autocrine stimulator of human gliomas. Sandberg-Nordqvist et al., 1993, *Cancer Res.* 53:2475-2478. The importance of the IGF-IR and its modulators in cell proliferation is further supported by the fact that many cell types in culture (fibroblasts, epithelial cells, smooth muscle cells, T-lymphocytes, myeloid cells, chondrocytes, osteoblasts, the stem cells of the bone marrow) are stimulated to grow by IGF-I. Goldring and Goldring, 1991, *Eukaryotic Gene Expression* 1:301-326. In a series of recent publications suggest that IGF-IR plays a central role in the mechanisms of transformation and, as such, could be a preferred target for therapeutic interventions for a broad spectrum of human malignancies. Baserga, 1995, *Cancer Res.* 55:249-252; Baserga, 1994, *Cell* 79:927-930; Coppola et al., 1994, *Mol. Cell. Biol.* 14:4588-4595.

The association between abnormalities in receptor PTKs and disease are not restricted to cancer, however. For example, receptor PTKs are associated with metabolic diseases like psoriasis, diabetes mellitus, wound healing, inflammation, and neurodegenerative diseases. EGF-R is indicated in corneal and dermal wound healing.

Defects in Insulin-R and IGF-IR are indicated in type-II diabetes mellitus. A more complete correlation between specific receptor PTKs and their therapeutic indications is set forth in Plowman et al., 1994, *DN&P* 7:334-339.

5 Non-receptor PTKs, including src, abl, fps, yes, fyn, lyn, lck, blk, hck, fgr, yrk (reviewed by Bolen et al., 1992, *FASEB J.* 6:3403-3409), are involved in the proliferative and metabolic signal transduction pathways also associated with receptor PTKs. Therefore, the  
10 present invention is also directed towards designing modulators against this class of PTKs. For example, mutated src (v-src) is an oncoprotein (pp60<sup>v-src</sup>) in chicken. Moreover, its cellular homolog, the proto-oncogene pp60<sup>c-src</sup> transmits oncogenic signals of many  
15 receptors. For example, over-expression of EGF-R or HER2/neu in tumors leads to the constitutive activation of pp60<sup>c-src</sup>, which is characteristic of the malignant cell but absent in the normal cell. On the other hand, mice deficient for the expression of c-src exhibit an  
20 osteopetrotic phenotype, indicating a key participation of c-src in osteoclast function and a possible involvement in related disorders. Similarly, Zap 70 is implicated in T-cell signaling. Both receptor PTKs and non-receptor PTKs are connected to hyperimmune  
25 disorders.

The instant invention is directed in part towards designing modulators of PTK function that could indirectly kill tumors by cutting off their source of sustenance. Normal vasculogenesis and angiogenesis play  
30 important roles in a variety of physiological processes such as embryonic development, wound healing, organ

regeneration and female reproductive processes such as follicle development in the corpus luteum during ovulation and placental growth after pregnancy. Folkman and Shing, 1992, *J. Biological Chem.* 267:10931-34.

5 However, many diseases are driven by persistent unregulated or inappropriate angiogenesis. For example, in arthritis, new capillary blood vessels invade the joint and destroy the cartilage. In diabetes, new capillaries in the retina invade the vitreous, bleed and  
10 cause blindness. Folkman, 1987, in: *Congress of Thrombosis and Haemostasis* (Verstraete, et. al, eds.), Leuven University Press, Leuven, pp.583-596. Ocular neovascularization is the most common cause of blindness and dominates approximately twenty (20) eye diseases.

15 Moreover, vasculogenesis and/or angiogenesis can be associated with the growth of malignant solid tumors and metastasis. A tumor must continuously stimulate the growth of new capillary blood vessels for the tumor itself to grow. Furthermore, the new blood vessels  
20 embedded in a tumor provide a gateway for tumor cells to enter the circulation and to metastasize to distant sites in the body. Folkman, 1990, *J. Natl. Cancer Inst.* 82:4-6; Klagsbrunn and Soker, 1993, *Current Biology* 3:699-702; Folkman, 1991, *J. Natl., Cancer Inst.* 82:4-6;  
25 Weidner et al., 1991, *New Engl. J. Med.* 324:1-5.

Several polypeptides with *in vitro* endothelial cell growth promoting activity have been identified. Examples include acidic and basic fibroblastic growth factor ( $\alpha$ FGF,  $\beta$ FGF), vascular endothelial growth factor  
30 (VEGF) and placental growth factor. Unlike  $\alpha$ FGF and  $\beta$ FGF, VEGF has recently been reported to be an

endothelial cell specific mitogen. Ferrara and Henzel, 1989, *Biochem. Biophys. Res. Comm.* 161:851-858; Vaisman et al., 1990, *J. Biol. Chem.* 265:19461-19566.

Thus, identifying the specific receptors that bind  
5 FGF or VEGF is important for understanding endothelial cell proliferation regulation. Two structurally related receptor PTKs that bind VEGF with high affinity are identified: the flt-1 receptor (Shibuya et al., 1990, *Oncogene* 5:519-524; De Vries et al., 1992, *Science* 10 255:989-991) and the KDR/FLK-1 receptor, discussed in the U.S. Patent Application No. 08/193,829. In addition, a receptor that binds  $\alpha$ FGF and  $\beta$ FGF is identified. Jaye et al., 1992, *Biochem. Biophys. Acta* 1135:185-199). Consequently, these receptor PTKs most  
15 likely regulate endothelial cell proliferation.

FGFRs play important roles in angiogenesis, wound healing, embryonic development, and malignant transformation. Basilico and Moscatelli, 1992, *Adv. Cancer Res.* 59:115-165. Four mammalian FGFR (FGFR1-4) have been described and additional diversity is  
20 generated by alternative RNA splicing within the extracellular domains. Jaye et al., 1992, *Biochem. Biophys. Acta* 1135:185-199. Like other receptor PTKs, dimerization of FGF receptors is essential for their  
25 activation. Soluble or cell surface-bound heparin sulfate proteoglycans act in concert with FGF to induce dimerization (Schlessinger et al., 1995, *Cell* 83:357-360), which leads to autophosphorylation of specific tyrosine residues in the cytoplasmic domain. Mohammadi  
30 et al., 1996, *Mol. Cell Biol.* 16:977-989.

Mutations in three human FGF receptor genes, FGFR1,

FGFR2, and FGFR3, have been implicated in a variety of human genetic skeletal disorders. Mutations in FGFR1 and FGFR2 result in the premature fusion of the flat bones of the skull and cause the craniosynostosis syndromes, such as Apert (FGFR2) (Wilkie et al., 1994, Nat. Genet. 8:269-274), Pfeiffer (FGFR1 and FGFR2) (Muenke et al., 1994, Nat. Genet. 8:269-274), Jackson-Weiss (FGFR2) (Jabs et al., 1994, Nat. Genet. 8:275-279) and Crouzon (FGFR2) (Jabs et al., 1994, Nat. Genet. 8:275-279) syndromes. In contrast mutations in FGFR3 are implicated in long bone disorders and cause several clinically related forms of dwarfism including achondroplasia (Shiang et al., 1994, Cell 78:335-342), hypochondroplasia (Bellus et al., 1995, Nat. Genet. 10:357-359) and the neonatal lethal thanatophoric dysplasia (Tavormina et al., 1995, Nat. Genet. 9:321-328). It has been shown that these mutations lead to constitutive activation of the tyrosine kinase activity of FGFR3 (Webster et al., 1996, EMBO J. 15:520-527). Furthermore gene-targeting experiments in mice have revealed an essential role for FGFR3 in developmental bone formation (Deng et al., 1996, Cell 84:911-921).

Another major role proposed for FGFs *in vivo* is the induction of angiogenesis (Folkman and Klagsbrun, 1987, Science 236:442). Therefore, inappropriate expression of FGFs or of their receptors or aberrant function of the tyrosine kinase activity could contribute to several human angiogenic pathologies such as diabetic retinopathy, rheumatoid arthritis, atherosclerosis and tumor neovascularization (Klagsbrun and Edelman, 1989, Arteriosclerosis 9:269). Moreover, FGFs are thought to

be involved in malignant transformation. Indeed, the genes coding for the three FGF homologues int-2, FGF-5 and hst-1/K-fgf were originally isolated as oncogenes. Furthermore, the cDNA encoding FGFR1 and FGFR2 are amplified in a population of breast cancers (Adnane et al., 1991, *Oncogene* 6:659-663). Over-expression of FGF receptors has been also detected in human pancreatic cancers, astrocytomas, salivary gland adenomasarcomas, Kaposi sarcomas, ovarian cancers and prostate cancers.

Evidence, such as the disclosure set forth in copending U.S. Application Serial No. 08/193,829, strongly suggests that VEGF is not only responsible for endothelial cell proliferation, but also is a prime regulator of normal and pathological angiogenesis. See generally, Klagsburn and Soker, 1993, *Current Biology* 3:699-702; Houck et al., 1992, *J. Biol. Chem.* 267:26031-26037. Moreover, it has been shown that KDR/FLK-1 and flt-1 are abundantly expressed in the proliferating endothelial cells of a growing tumor, but not in the surrounding quiescent endothelial cells. Plate et al., 1992, *Nature* 359:845-848; Shweiki et al., 1992, *Nature* 359:843-845.

The invention is directed to designing and identifying modulators of receptor and non-receptor PTK functions that could modify the inappropriate activity of a PTK involved with a clinical disorder. The rational design and identification of modulators of PTK functions can be accomplished by utilizing the structural coordinates that define a PTK three dimensional structure.

## II. Modulators of PTK functions as Therapeutics for Disease

As a consequence of the disorders discussed above, scientists in the biomedical community are searching for modulators of PTK functions that down-regulate signal transduction pathways associated with inappropriate PTK activity.

In particular, small molecule modulators of PTK functions are sought as some can traverse the cell membrane and do not hydrolyze in acidic environments. Some compounds have already been discovered. For example, bis monocyclic, bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808) 1-cyclopropyl-4-pyridyl-quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 A1), seleoindoles and selenides (PCT WO 94/03427), tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although some modulators of PTK function are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the oxindolinone/thiolindolinone family, however, are specific for the FGF receptor subfamily (U.S. Patent Application Serial No. 08/702,232, filed August 23, 1996, invented by Tang et al., entitled "Indolinone Combinatorial Libraries and Related Products and Methods for the Treatment of

Disease," Attorney Docket No. 221/187). In addition, compounds of the oxindolinone/thiolindolinone family are non-hydrolyzable in acidic conditions and can be highly bioavailable.

5       The invention provides information regarding the specific interactions between a PTK and compounds of the oxindolinone/thiolindolinone family. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, the PTKs in these structures are not complexed with PTK subfamily specific, hydrolysis resistant, highly bioavailable small molecules. The X-ray crystallography techniques used in the current invention resolve interactions between a PTK and compounds in complex with it at the atomic level, which provides detailed information regarding the orientation of chemical groups defining an effective modulator of PTK function.

### 15       III. Crystalline Tyrosine Kinases

20       Crystalline PTKs of the invention include native crystals, derivative crystals and co-crystals. The native crystals of the invention generally comprise substantially pure polypeptides corresponding to the tyrosine kinase domain in crystalline form.

25       It is to be understood that the crystalline tyrosine kinase domains of the invention are not limited to naturally occurring or native tyrosine kinase domains. Indeed, the crystals of the invention include mutants of native tyrosine kinase domains. Mutants of native tyrosine kinase domains are obtained by replacing at least one amino acid residue in a native tyrosine

30



kinase domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C-terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native tyrosine kinase domain from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root-mean-square deviation of less than or equal to about 2Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the Cα atoms of the native tyrosine kinase domain are included in the superposition.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the tyrosine kinase domain will depend, in part, on the region of the tyrosine kinase domain where the substitution, addition or deletion occurs. In highly variable regions of the molecule, such as those shown in FIG. 6, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, such as those regions shown in FIG. 6, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are well-known in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility,

hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids  
5 include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative  
10 amino acid substitutions are well known in the art.

For tyrosine kinase domains obtained in whole or in part by chemical synthesis, the selection of amino acids available for substitution or addition is not limited to the genetically encoded amino acids. Indeed, the  
15 mutants described herein may contain non-genetically encoded amino acids. Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other amino acids  
20 can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or  
25 add amino acid residues to a native tyrosine kinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, and for crystallization of the polypeptide. Such substitutions, deletions and/or  
30 additions which do not substantially alter the three dimensional structure of the native tyrosine kinase

domain will be apparent to those of ordinary skill in the art.

It should be noted that the mutants contemplated herein need not exhibit PTK activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the tyrosine kinase domain but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated tyrosine kinase domain. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold, mercury, etc.

The co-crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc.

#### IV. Three Dimensional Structure Determination Using X-ray Crystallography

X-ray crystallography is a method of solving the three dimensional structures of molecules. The structure of a molecule is calculated from X-ray diffraction patterns using a crystal as a diffraction grating. Three dimensional structures of protein molecules arise from crystals grown from a concentrated aqueous solution of that protein. The process of X-ray crystallography can include the following steps:

- (a) synthesizing and isolating a polypeptide;
- (b) growing a crystal from an aqueous solution comprising the polypeptide with or without a modulator; and
- (c) collecting X-ray diffraction patterns from the crystals, determining unit cell dimensions and symmetry, determining electron density, fitting the amino acid sequence of the polypeptide to the electron density, and refining the structure.

#### Production of Polypeptides

The native and mutated tyrosine kinase domain polypeptides described herein may be chemically synthesized in whole or part using techniques that are well-known in the art (see, e.g., Creighton, 1983). Alternatively, methods which are well known to those skilled in the art can be used to construct expression vectors containing the native or mutated tyrosine kinase domain polypeptide coding sequence and appropriate

transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques and *in vivo* recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989 and Ausubel et al., 1989.

A variety of host-expression vector systems may be utilized to express the tyrosine kinase domain coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the tyrosine kinase domain coding sequence; yeast transformed with recombinant yeast expression vectors containing the tyrosine kinase domain coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing the tyrosine kinase domain coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the tyrosine kinase domain coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage  $\lambda$ , plac, ptrp,

ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when generating cell lines that contain multiple copies of the tyrosine kinase domain DNA, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

Methods describing methods of DNA manipulation, vectors, various types of cells used, methods of incorporating the vectors into the cells, expression techniques, protein purification and isolation methods, and protein concentration methods are disclosed in detail with respect to the protein PYK-2 in PCT publication WO 96/18738. This publication is incorporated herein by reference in its entirety, including any drawings. Those skilled in the art will appreciate that such descriptions are applicable to the present invention and can be easily adapted to it.

Crystal Growth

Crystals are grown from an aqueous solution containing the purified and concentrated polypeptide by a variety of techniques. These techniques include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. McPherson, 1982, John Wiley, New York; McPherson, 1990, *Eur. J. Biochem.* 189:1-23; Webber, 1991, *Adv. Protein Chem.* 41:1-36, incorporated by reference herein in its entirety, including all figures, tables, and drawings.

Generally, the native crystals of the invention are grown by adding precipitants to the concentrated solution of the polypeptide corresponding to the PTK catalytic domain. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

For crystals of the invention, it has been found that hanging drops containing about 2.0  $\mu$ L of tyrosine kinase domain polypeptide (10 mg/mL in 10mM Tris-HCl, pH 8.0, 10 mM NaCl and 2 mM dithiothreitol) and 2.0  $\mu$ L reservoir solution (16% w/v polyethylene glycol MW 10000, 0.3 M  $(\text{NH}_4)_2\text{SO}_4$ , 5% v/v ethylene glycol or glycerol and 100 mM bis-Tris, pH 6.5) suspended over 0.5 mL reservoir buffer for about 3-4 weeks at 4°C provide crystals suitable for high resolution X-ray structure determination.

Those of ordinary skill in the art will recognize that the above-described crystallization conditions can be varied. Such variations may be used alone or in

combination, and include polypeptide solutions containing polypeptide concentrations between about 1 mg/mL and about 60 mg/mL, Tris-HCl concentrations between about 10 mM and about 200 mM, dithiothreitol concentrations between about 0 mM and about 20 mM, pH ranges between about 5.5 and about 7.5; and reservoir solutions containing polyethylene glycol concentrations between about 10% and about 30% (w/v), polyethylene glycol molecular weights between about 1000 and about 20,000,  $(\text{NH}_4)_2\text{SO}_4$  concentrations between about 0.1 M and about 0.5 M, ethylene glycol or glycerol concentrations between about 0% and about 20% (v/v), bis-Tris concentrations between about 10 mM and about 200 mM, pH ranges between about 5.5 and about 7.5 and temperature ranges between about 0° C and about 25°C. Other buffer solutions may be used such as HEPES buffer, so long as the desired pH range is maintained.

Derivative crystals of the invention can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. It has been found that soaking a native crystal in a solution containing about 0.1 mM to about 5 mM thimerosal, 4-chloromeruribenzoic acid or  $\text{KAu}(\text{CN})_2$  for about 2 hr to about 72 hr provides derivative crystals suitable for use as isomorphous replacements in determining the X-ray crystal structure of the tyrosine kinase domain polypeptide.

Co-crystals of the invention can be obtained by soaking a native crystal in mother liquor containing compound that bind the kinase domain, or described above, or can be obtained by co-crystallizing the kinase



domain polypeptide in the presence of one or more binding compounds.

For co-crystals of tyrosine kinase domain polypeptide in co-complex with AMP-PCP, it has been found that co-crystallizing the kinase domain polypeptide in the presence of AMP-PCP using the above-described crystallization conditions for obtaining native crystals with a polypeptide solution additionally containing 10 mM AMP-PCP and 20 mM  $MgCl_2$  yields co-crystals suitable for the high resolution structure determination by X-ray crystallography. Of course, those having skill in the art will recognize that the concentrations of AMP-PCP and  $MgCl_2$  in the polypeptide solution can be varied, alone or in combination with the variations described above for native crystals. Such variations include polypeptide solutions containing AMP-PCP concentrations between 0.1 mM and 50 mM and  $MgCl_2$  concentrations between 0 mM and 50 mM.

Crystals comprising a polypeptide corresponding to a PTK catalytic domain complexed with a compound can be grown by one of two methods. In the first method, the modulator is added to the aqueous solution containing the polypeptide corresponding to the PTK catalytic domain before the crystal is grown. In the second method, the modulator is soaked into an already existing crystal of a polypeptide corresponding to a PTK catalytic domain.

Crystalline FGFR

In one illustrative embodiment, the invention provides crystals of FGFR1. The crystals were obtained by the methods provided in the Examples. The FGFR1 crystals, which may be native crystals, derivative crystals or co-crystals, have monoclinic unit cells (*i.e.*, unit cells wherein  $a \neq b \neq c$ ;  $\alpha = \gamma = 90^\circ$ ; and  $\beta > 90^\circ$ ) and space group symmetry C2. There are two FGFR1 molecules in the asymmetric unit, related by an approximate two-fold axis.

Two forms of crystalline FGFR1 were obtained. In one form (designated "C2-A form"), the unit cell has dimensions of  $a = 208.3 \text{ \AA}$ ,  $b = 57.2 \text{ \AA}$ ,  $c = 65.5 \text{ \AA}$  and  $\beta = 107.2^\circ$ . In another form (designated "C2-B form"), the unit cell has dimensions of  $a = 211.6 \text{ \AA}$ ,  $b = 51.3 \text{ \AA}$ ,  $c = 66.1 \text{ \AA}$  and  $\beta = 107.7^\circ$ .

Three distinct two-fold related FGFR1 dimers are observed in both the C2-A and C2-B forms of the FGFR1 crystal, one non-crystallographically related dimer and two crystallographically related dimers. The non-crystallographically related dimer comprises the two molecules in the asymmetric unit. The residues making up the dimer interface are located in C-terminal lobe. In this dimer, the C-terminal lobes abut with the N-terminal lobes distal to one another. The total amount of surface area buried in the surface is about  $950 \text{ \AA}^2$ . Very few of the interactions in the interface are of a specific nature, *e.g.*, hydrogen-bonding or close packing of hydrophobic residues.

There are two crystallographically-related dimers in the C2 lattice. In the first dimer, the residues

that constitute the dimer interface are limited to those in the  $\beta$ -sheet of the N-terminal lobe (amino acid residues 477, 479, 498, 506, 508 and 496). The total surface area buried in this interface is about 670 Å<sup>2</sup>.

5 The interactions are rather specific. Three hydrophobic residues which are partially solvent-exposed in the monomer, Val-479, Ile-498 and Val-508, come together with their two-fold-related residues to form a compact hydrophobic plug. This plug is capped on either side by  
10 a salt bridge between Arg-477 and Glu-496. In addition, two main-chain hydrogen-bonds connect the  $\beta$ -sheets of the two monomers at the start of  $\beta$ 3 (amino acid residues 506 and 508). The residues in this dimer interface, or their residue character, are generally conserved in the  
15 mammalian FGF receptors, but not in the invertebrate homologues.

The other crystallographically-related dimer buries about 1650 Å<sup>2</sup> in its interface. In this dimer, the  $\alpha$ C helices of the two monomers are nearly parallel and  
20 contact each other at their C-terminal ends. Met-534 and Met-537 are in van der Waals contact with their two-fold-related residues. Other hydrophobic contacts involve Pro-466 with Ile-648 and Pro-469 with Ile-676 and Thr-678. In addition, hydrogen bonds (side-chain to  
25 main-chain) are made between Arg-470 and Lys-618 and between His-649 and Glu-464, and there are several water molecules that bridge the two monomers through hydrogen bonding.

In the C2-B form of the crystal, the monomers of  
30 this second crystallographically-related dimer are shifted slightly with respect to one another (6°

rotation), indicating that this interface is somewhat fluid.

In both of the crystallographically-related dimers, the N-termini of the two molecules comprising the dimer point in the same direction and are reasonably close to one another.

Determining Unit Cell Dimensions and the Three Dimensional Structure of a Polypeptide or Polypeptide Complex

Once the crystal is grown, it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection device. Collection of X-ray diffraction patterns are well documented by those in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. A beam of X-rays enter the crystal and then diffract from the crystal. An X-ray detection device can be utilized to record the diffraction patterns emanating from the crystal. Although the X-ray detection device on older models of these instruments is a piece of film, modern instruments digitally record X-ray diffraction scattering.

Methods for obtaining the three dimensional structure of the crystalline form of a peptide molecule or molecule complex are well known in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. The following are steps in the process of determining the three dimensional structure of a molecule or complex from X-ray diffraction data.

After the X-ray diffraction patterns are collected from the crystal, the unit cell dimensions and orientation in the crystal can be determined. They can be determined from the spacing between the diffraction emissions as well as the patterns made from these emissions. The unit cell dimensions are characterized in three dimensions in units of Angstroms (one Å =  $10^{-10}$  meters) and by angles at each vertices. The symmetry of the unit cell in the crystals is also characterized at this stage. The symmetry of the unit cell in the crystal simplifies the complexity of the collected data by identifying repeating patterns. Application of the symmetry and dimensions of the unit cell is described below.

Each diffraction pattern emission is characterized as a vector and the data collected at this stage of the method determines the amplitude of each vector. The phases of the vectors can be determined using multiple techniques. In one method, heavy atoms can be soaked into a crystal, a method called isomorphous replacement, and the phases of the vectors can be determined by using these heavy atoms as reference points in the X-ray analysis. Otwinowski, 1991, Daresbury, United Kingdom, 80-86. The isomorphous replacement method usually requires more than one heavy atom derivative. In another method, the amplitudes and phases of vectors from a crystalline polypeptide with an already determined structure can be applied to the amplitudes of the vectors from a crystalline polypeptide of unknown structure and consequently determine the phases of these vectors. This second method is known as molecular

replacement and the protein structure which is used as a reference must have a closely related structure to the protein of interest. Naraza, 1994, *Proteins* 11:281-296. Thus, the vector information from a PTK of known  
5 structure, such as those reported herein, are useful for the molecular replacement analysis of another PTK with unknown structure.

Once the phases of the vectors describing the unit cell of a crystal are determined, the vector amplitudes and phases, unit cell dimensions, and unit cell symmetry  
10 can be used as terms in a Fourier transform function. The Fourier transform function calculates the electron density in the unit cell from these measurements. The electron density that describes one of the molecules or  
15 one of the molecule complexes in the unit cell can be referred to as an electron density map. The amino acid structures of the sequence or the molecular structures of compounds complexed with the crystalline polypeptide may then fit to the electron density using a variety of  
20 computer programs. This step of the process is sometimes referred to as model building and can be accomplished by using computer programs such as TOM/FRODO. Jones, 1985, *Methods in Enzymology* 115:157-171.

25 A theoretical electron density map can then be calculated from the amino acid structures fit to the experimentally determined electron density. The theoretical and experimental electron density maps can be compared to one another and the agreement between  
30 these two maps can be described by a parameter called an R-factor. A low value for an R-factor describes a high

degree of overlapping electron density between a theoretical and experimental electron density map.

The *R*-factor is then minimized by using computer programs that refine the theoretical electron density map. A computer program such as X-PLOR can be used for model refinement by those skilled in the art. Brünger, 1992, *Nature* 355:472-475. Refinement may be achieved in an iterative process. A first step can entail altering the conformation of atoms defined in an electron density map. The conformations of the atoms can be altered by simulating a rise in temperature which will increase the vibrational frequency of the bonds and modify positions of atoms in the structure. At a particular point in the atomic perturbation process, a force field, which typically defines interactions between atoms in terms of allowed bond angles and bond lengths, Van der Waals interactions, hydrogen bonds, ionic interactions, and hydrophobic interactions, can be applied to the system of atoms. Favorable interactions may be described in terms of free energy and the atoms can be moved over many iterations until a free energy minimum is achieved. The refinement process can be iterated until the *R*-factor reaches a minimum value.

The three dimensional structure of the molecule or molecule complex is described by atoms that fit the theoretical electron density characterized by a minimum *R*-value. A file can then be created for the three dimensional structure that defines each atom by coordinates in three dimensions. Examples of such structural coordinate files are defined in Table 1, Table 2, Table 3, and Table 4.

V. Structures of FGFR1

The present invention provides high-resolution three-dimensional structures and atomic structure coordinates of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the examples. The atomic structure coordinates of crystalline FGFR1, obtained from the C2-A form of the crystal to 2.0 Å resolution, are listed in Table 3; the coordinates of crystalline FGFR1:AMP-PCP co-complex, obtained from the C2-A form of the crystal to 2.3 Å resolution are listed in Table 4.

Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of FGFR1, whether native crystals, derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 1.5 Å when superimposed, using backbone atoms (N, C $\alpha$ , C and O), on the structure coordinates listed in Table 3 or Table 4 are considered to be identical with the structure coordinates listed in the Tables when at least about 50% to 100% of the backbone atoms of FGFR1 are included in the superposition.

Referring now to FIG. 1, the overall structure of FGFR1 is bi-lobate. The N-terminal lobe of FGFR1 spans amino acid residues 456-567 (FIG. 3) and comprises a curled  $\beta$ -sheet of five anti-parallel strands ( $\beta$ 1- $\beta$ 5) and



one  $\alpha$ -helix ( $\alpha$ C). The C-terminal lobe spans amino acid residues 568-765 (FIG. 3) and comprises two  $\beta$ -strands ( $\beta$ 7,  $\beta$ 8) and seven  $\alpha$ -helices ( $\alpha$ D,  $\alpha$ E,  $\alpha$ EF,  $\alpha$ F- $\alpha$ I). The secondary structure nomenclature follows that used for IRK (Hubbard et al., 1994) which in turn is based on the assignments for cAPK (Knighton et al., 1991). FIG. 2 shows a stereo view of a  $C_\alpha$  trace of FGFR1 in the same orientation as FIG. 1.

A structure-based sequence alignment of the tyrosine kinase domains of human fibroblast growth factor receptor 1 (human FGFR1; labelled FGFR1), human fibroblast growth factor receptors 2, 3 and 4 (labelled FGFR2, FGFR3 and FGFR4, respectively), a *D. melanogaster* homologue (labelled DFDFR1), a *C. elegans* homologue (labelled EGL-15) and insulin receptor kinase (labelled IRK), is shown in FIG. 3. The sequence of FGFR1, which is not shown in FIG. 3 is identical to the sequence of FGFR1 except that FGFR1 has the following amino acid substitutions and additions: Cys-488  $\rightarrow$  Ala, Cys-584  $\rightarrow$  Ser, Leu-457  $\rightarrow$  Val and an additional five N-terminal amino acids (Ser-Ala-Ala-Gly-Thr). The secondary structure assignments for FGFR1 and IRK were obtained using the Kabsch and Sander algorithm (Kabsch and Sander, 1983) as implemented in PROCHECK (Laskowski et al., 1993). In the FGF receptor sequences, a period represents sequence identity to FGFR1. In the IRK sequence, residues that are identical to FGFR1 are highlighted. A hyphen denotes an insertion.

The numbers under the EGL-15 sequence represent the fractional solvent accessibility (FSA2) of the residue in the FGFR1 structure. The FSA ratio is the ratio of

the solvent-accessible surface area of a residue in a Gly-X-Gly tripeptide compared to that in the FGFR1 structure. A value of 0 represents an FSA between 0.00 and 0.09; 1 represents an FSA between 0.10 and 0.19, etc. The higher the value, the more solvent-exposed the residue. An asterisk or pound sign in the FSA line indicates that the residue (asterisk) or side chain (pound sign) is not included in the atom model due to disorder. The numbers below the FSA line are the FSAs for those residues that form part of a dimer interface.

The amino acid residue numbers for FGFR1, and hence FGFR1, and IRK provided in FIG. 3 are used in the discussion that follows. Significant differences in the N-terminal lobe of FGFR1 as compared to IRK are found in the loops between  $\beta$  strands and in  $\alpha$ C. Residues from the end of  $\beta$ 1 through the beginning of  $\beta$ 2 (amino acid residues 485-490) form the nucleotide-binding loop, named because of its role in ATP coordination. This residue stretch contains the protein kinase-conserved GXGXXG sequence motif, where X is any amino acid. This loop is poorly ordered in one FGFR1 molecule in the asymmetric unit and disordered (*i.e.*, not included in the atomic model) in the other FGFR1 molecule in the asymmetric unit. The loop between  $\beta$ 1 and  $\beta$ 3 is disordered in both FGFR1 molecules comprising the asymmetric unit.

Referring now to FIG. 4A, which provides a ribbon diagram of the N-terminal lobes of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\beta$ -sheets have been superimposed, it can be seen that in FGFR1  $\alpha$ C is longer by one helical turn than in IRK and is oriented such

that residues Lys-514 and Glu-531, which are conserved in protein kinases, form a salt bridge (represented by a black line). While not intending to be bound by theory, this salt bridge is believed to be important for proper positioning of the conserved lysine side chain, which coordinates two phosphate oxygens of ATP. The salt bridge is observed in the structures of cAPK (Knighton et al., 1991) and mitogen-activated protein kinase (MAPK) (Zhang et al., 1994).

Referring now to FIG. 4B, which provides a ribbon diagram of the C-terminal lobes of FGFR1 and IRK in which the C $\alpha$  atoms of the  $\alpha$ -helices have been superimposed, a significant difference is found in the C-terminal helix of FGFR1 when compared to IRK; helix  $\alpha$ I of FGFR1 is longer by seven residues (two helical turns) than its counterpart in IRK. The extended length of  $\alpha$ I is presumably important in the biological functioning of FGF receptors, since the tyrosine autophosphorylation site to which an SH2 domain of PLC $\gamma$  binds is six residues C-terminal to this helix.

The structure of FGFR1 displays an open disposition of the N- and C-terminal lobes. Despite having different sets of lattice contacts, the two FGFR1 molecules in the asymmetric unit have only a 2° difference in relative lobe orientation. It appears as though the steric interaction between residues in  $\alpha$ C (Glu-531 and Met-534) with Phe-642 and Gly-643 of the protein kinase-conserved DFG sequence at the beginning of the activation loop accounts for the open conformation of FGFR1.

The active site of FGFR1 is characterized by at

least amino acid residues spanning the catalytic loop, activation loop and nucleotide binding loop. Unlike the structure of IRK, in which Tyr-1162 occupies the active site of the molecule, the active sites of both FGFR1  
5 molecules in the asymmetric unit are unoccupied.

The activation loop, which regulates phosphorylation, is characterized by at least residues 640 to 663. Quite surprisingly, while the activation loops of FGFR1 and IRK contain the same number of amino  
10 acid residues and share greater than 50% sequence homology, the paths of the polypeptide chains are strikingly dissimilar, diverging at Ala-640 (Gly-1149 in IRK) and reconverging at Val-664 (Val-1173 in IRK). Tyr-653 and Tyr 564 are not bound in the active site.  
15 Instead, these residues point away from it. Tyr-653 is in van der Waals contact with several hydrophobic residues (Val-664, Leu-672 and Phe-710) and is hydrogen-bonded via its hydroxyl group to a backbone carbonyl oxygen (Leu-672). Tyr-654 is more solvent exposed than  
20 Tyr-653, and its only van der Waals contact is with Val-706. Temperature factor data suggest that the activation loop is relatively mobile and adopts multiple conformations.

The catalytic loop of protein kinases lies between  
25 secondary structure elements  $\alpha E$  and  $\beta 7$  and contains an invariant aspartic acid residue (Asp-623 in FGFR1) which serves as the catalytic base in the phosphotransfer reaction, abstracting the proton from the hydroxyl group of the substrate tyrosine, serine or threonine. The  
30 catalytic loop sequence of FGFR1 comprises at least residues His-621 to Asn-628 (amino acid sequence

HRDLAARN), and is identical to that for IRK and most receptor and non-receptor PTKs.

In addition to the two tyrosine autophosphorylation sites in the activation loop (Tyr-653 and Tyr-654), there are four other autophosphorylation sites present in the FGFR1 crystals of the invention: one in the juxtamembrane region (Tyr-463), two in the kinase insert (Tyr-583 and Tyr-585) and one in the C-terminal lobe (Tyr-730) (Mohammadi et al., 1996). They exhibit varying degrees of conservation in mammalian FGF receptors: Tyr-463 and Tyr-585 in FGFR1 and 2; Tyr-583 in FGFR1, 2 and 3; and Tyr-730 in FGFR 1, 2, 3 and 4 (FIG. 3).

Referring now to FIG. 5, the positions of the autophosphorylation sites are mapped onto the FGFR1 structure. The juxtamembrane site (Tyr-463) and the residues N-terminal to it are disordered in one of the FGFR1 molecules in the asymmetric unit. In the other molecule in the asymmetric unit Tyr-463 is involved in a lattice contact.

The kinase insert region (the region between helices  $\alpha$ D and  $\alpha$ E) contains autophosphorylation sites Tyr-583 and Tyr-585 and is disordered in both FGFR1 molecules in the asymmetric unit of the C2-A form of the crystal. In the C2-B form, several lattice contacts partially pin down this region in one of the two FGFR1 molecules in the asymmetric unit, allowing a trace of the polypeptide chain to be made. There is no well-defined secondary structure for these residues. Tyr-730, situated in  $\alpha$ H in the C-terminal lobe, is nearly buried and the side-chain hydroxyl group makes two

hydrogen-bonds. The side chains of neighboring Met-732 and Met-733 are both buried. Therefore, phosphorylation of Tyr-730 would presumably require prior unfolding of  $\alpha$ H.

5        Aside from Tyr-730, the five other autophosphorylation sites (including Tyr-653 and Tyr-654) are found in relatively mobile segments of the FGFR1 molecule. While not intending to be bound by theory, the spatial positions of the autophosphorylation sites relative to the active site suggest that autophosphorylation occurs by a *trans* mechanism between  
10       two kinase domains, supporting the hypothesis that ligand-induced receptor dimerization is critical for the initiation of autophosphorylation events.

15       The structure of crystalline FGFR1:AMP-PCP co-complex is essentially similar to that observed for crystalline FGFR1. There are no significant changes in the structure of FGFR1 induced by AMP-PCP binding. In particular, binding of AMP-PCP, and by extension ATP, does not by itself promote lobe closure under the  
20       crystallization conditions used. Furthermore, complexation did not result in any noticeable changes in the conformations of the activation and nucleotide-binding loops.

25       The crystalline FGFR1:AMP-PCP co-complex contains hydrogen bonds that are present between N1 of adenine and the amide nitrogen of Ala-564 and between N6 of adenine and the carbonyl oxygen of Glu-562. The adenine ring is flanked on one side by Leu-484 and Val-492 (N-terminal lobe) and on the other side by Leu-630  
30       (C-terminal lobe). The ribose hydroxyl groups make no

direct hydrogen bonds with protein atoms. Lys-514 is hydrogen-bonded to oxygens of the  $\beta$ - and  $\gamma$ -phosphates.

There is no unambiguous electron density that would indicate the positions of  $Mg^{2+}$  ions. Generally, AMP-PCP appears to be coordinated rather loosely to unphosphorylated FGFR1, being bound to the "roof" of the cleft rather than being tightly sandwiched between the two kinase lobes.

#### 10 Structural Differences Between FGF-R and IRK

Several features distinguish the FGF-receptor structure from that of the insulin-receptor tyrosine kinase. These distinctions are likely to be important in signaling by FGF-receptors, and other monomeric receptors that are believed to undergo ligand-induced dimerization.

The most significant difference between the structures of FGFR1 and IRK is the conformation of the activation loop. In FGFR1, the activation loop is disposed such that the binding site for substrate peptides is blocked not by an activation loop tyrosine, as in IRK, but by Arg-661 and PTK-invariant Pro-663, while the ATP binding site is accessible. This represents another molecular mechanism by which a receptor PTK may be autoinhibited. The observed autoinhibition in FGFR1 would appear to be weaker than that in IRK because of fewer specific interactions made by residues in the FGFR1 activation loop (manifested in the relatively higher B-values) and the accessibility of the ATP site. One obvious distinction between the insulin and FGF receptor families is that in the former,

receptors are covalently linked heterotetramers ( $\alpha_2\beta_2$ ), whereas in the latter, receptor dimerization is ligand dependent. Receptors whose kinase domains are always in close proximity may require a stronger autoinhibition mechanism than those receptors that associate only upon ligand binding (Taylor et al., 1995). Since most growth factor receptors undergo ligand-dependent dimerization and activation, the FGF receptor autoinhibition mechanism appears to be a more general one.

#### VI. Uses of the Crystals and Atomic Structure Coordinates

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals described herein can be used as a starting material in any of the art-known methods of use for receptor and non-receptor tyrosine kinases. Such methods of use include, for example, identifying molecules that bind to the native or mutated catalytic domain of tyrosine kinases. The crystals and structure coordinates are particularly useful for identifying compounds that inhibit receptor and non-receptor tyrosine kinases as an approach towards developing new therapeutic agents (see, e.g., Levitzki and Gazit, 1995).

The structure coordinates described herein can be used as phasing models for determining the crystal structures of additional native or mutated tyrosine kinase domains, as well as the structures of co-crystals of such domains with ligands such as inhibitors, agonists, antagonists, and other molecules. The



structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated tyrosine kinase domains, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of receptor and non-receptor tyrosine kinases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific FGFR1 exemplary crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of the tyrosine kinase domain of any cytoplasmic tyrosine kinase that undergoes ligand-induced dimerization or receptor tyrosine kinase, including but not limited to the tyrosine kinases of FIG. 6.

#### VII. Structure Determination for PTKs with Unknown Structure Using Structural Coordinates

Structural coordinates, such as those set forth in Table 1, Table 2, Table 3, and Table 4, can be used to determine the three dimensional structures of PTKs with unknown structure. The methods described below can apply structural coordinates of a polypeptide with known structure to another data set, such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Preferred embodiments of the invention relate to determining the three dimensional structures of PTKs and related polypeptides. These include receptor PTKs such as FGF-

R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Non-receptor PTKs such as SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK can also be used in the methods described  
5 herein.

### Structures Using Amino Acid Homology

Homology modeling is a method of applying structural coordinates of a polypeptide of known  
10 structure to the amino acid sequence of a polypeptide of unknown structure. This method is accomplished using a computer representation of the three dimensional structure of a polypeptide or polypeptide complex, the computer representation of amino acid sequences of the polypeptides with known and unknown structures, and  
15 standard computer representations of the structures of amino acids. Homology modeling comprises the steps of (a) aligning the amino acid sequences of the polypeptides with and without known structure; (b)  
20 transferring the coordinates of the conserved amino acids in the known structure to the corresponding amino acids of the polypeptide of unknown structure; refining the subsequent three dimensional structure; and (d) constructing structures of the rest of the polypeptide.  
25 One skilled in the art recognizes that conserved amino acids between two proteins can be determined from the sequence alignment step in step (a).

The above method is well known to those skilled in the art. Greer, 1985, *Science* 228, 1055. Blundell et al., 1988, *Eur. J. Biochem.* 172, 513. A computer  
30 program currently utilized for homology modeling by

those skilled in the art is the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc.

5 Alignment of the amino acid sequence is accomplished by first placing the computer representation of the amino acid sequence of a polypeptide with known structure above the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous (e.g., amino acid side chains that are similar in chemical nature - aliphatic, aromatic, polar, or charged) are grouped together. This method will detect conserved regions of the polypeptides and account for amino acid insertions or deletions.

15 Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in the computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.

25 The structures of amino acids located in non-conserved regions are to be assigned manually by either using standard peptide geometries or molecular simulation techniques, such as molecular dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

30

The homology modeling method is well known to those skilled in the art and has been practiced using different protein molecules. The three dimensional structure of the polypeptide corresponding to the catalytic domain of a serine/threonine protein kinase, myosin light chain protein kinase, was homology modeled from the cAMP-dependent protein kinase catalytic subunit. Knighton et al., 1992, *Science* 258:130-135.

#### 10 Structures Using Molecular Replacement

Molecular replacement is a method of applying the X-ray diffraction data of a polypeptide of known structure to the X-ray diffraction data of a polypeptide of unknown sequence. This method can be utilized to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. X-PLOR is a commonly utilized computer software package used for molecular replacement. Brünger, 1992, *Nature* 355:472-475. AMORE is another program used for molecular replacement. Navaza, 1994, *Acta Crystallogr. A* 50:157-163. Preferably, the resulting structure does not exhibit a root-mean-square deviation of more than 3 Å.

25 A goal of molecular replacement is to align the positions of atoms in the unit cell by matching electron diffraction data from two crystals. A program such as X-PLOR can involve four steps. A first step can be to determine the number of molecules in the unit cell and define the angles between them. A second step can involve rotating the diffraction data to define the orientation of the molecules in the unit cell. A third

30

step can be to translate the electron density in three dimensions to correctly position the molecules in the unit cell. Once the amplitudes and phases of the X-ray diffraction data is determined, an R-factor can be calculated by comparing electron diffraction maps calculated experimentally from the reference data set and calculated from the new data set. An R-factor between 30-50% indicates that the orientations of the atoms in the unit cell are reasonably determined by this method. A fourth step in the process can be to decrease the R-factor to roughly 20% by refining the new electron density map using iterative refinement techniques described herein and known to those of ordinary skill in the art.

#### Structures Using NMR Data

Structural coordinates of a polypeptide or polypeptide complex derived from X-ray crystallographic techniques can be applied towards the elucidation of three dimensional structures of polypeptides from nuclear magnetic resonance (NMR) data. This method is used by those skilled in the art. Wuthrich, 1986, John Wiley and Sons, New York:176-199; Pflugrath et al., 1986, *J. Molecular Biology* 189:383-386; Kline et al., 1986, *J. Molecular Biology* 189:377-382. While the secondary structure of a polypeptide is often readily determined by utilizing two-dimensional NMR data, the spatial connections between individual pieces of secondary structure are not as readily determinable. The coordinates defining a three-dimensional structure of a polypeptide derived from X-ray crystallographic

techniques can guide the NMR spectroscopist to an understanding of these spatial interactions between secondary structural elements in a polypeptide of related structure.

5       The knowledge of spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. Additionally, applying the crystallographic coordinates after the determination of  
10       secondary structure by NMR techniques only simplifies the assignment of NOEs relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure. Conversely, using the crystallographic coordinates to  
15       simplify NOE data while determining secondary structure of the polypeptide would bias the NMR analysis of protein structure.

As the analysis of polypeptide structure by NMR methods is a relatively new technique, the use of  
20       structural coordinates defining a PTK structure will most likely be utilized more frequently in the near future. As the method progresses, the three dimensional structure analysis of polypeptides of the same size as a PTK catalytic domain will become more frequent.

25       VIII.       Structure-Based Design of Modulators of PTK Function Utilizing Structural Coordinates  
                  Structure-based modulator design and identification

30       methods are powerful techniques that can involve searches of computer data bases containing a wide variety of potential modulators and chemical functional

groups. The computerized design and identification of modulators is useful as the computer data bases contain more compounds than the chemical libraries, often by an order of magnitude. For reviews of structure-based drug design and identification see Kuntz et al., 1994, *Acc. Chem. Res.* 27:117; Guida, 1994, *Current Opinion in Struc. Biol.* 4: 777; Colman, 1994, *Current Opinion in Struc. Biol.* 4: 868.

The three dimensional structure of a polypeptide defined by structural coordinates can be utilized by these design methods. The structural coordinates of Table 1, Table 2, Table 3, and Table 4 can be utilized by this method. In addition, the three dimensional structures of receptor and non-receptor PTKs determined by the homology, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods. Thus, the structures of receptor PTKs, FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK, can be utilized by the methods described herein. The structures of non-receptor PTKs, SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK, can also be utilized by the rational modulator design method.

#### Design by Searching Molecular Data Bases

One method of rational modulator design searches for modulators by docking the computer representation of compounds from a data base of molecules. Publicly available data bases include:

- a) ACD from Molecular Designs Limited

- b) NCI from National Cancer Institute
- c) CCDC from Cambridge Crystallographic Data Center
- d) CAST from Chemical Abstract Service
- e) Derwent from Derwent Information Limited
- 5 f) Maybridge from Maybridge Chemical Company LTD
- g) Aldrich from Aldrich Chemical Company
- h) Directory of Natural Products from Chapman & Hall

One such data base (ACD distributed by Molecular Designs  
10 Limited Information Systems) contains, for example,  
200,000 compounds that are synthetically derived or are  
natural products. Methods available to those skilled in  
the art can convert a data set represented in two  
dimensions to one represented in three dimensions.  
15 These methods are enabled by such computer programs as  
CONCORD from Tripos Associates or DB-Converter from  
Molecular Simulations Limited.

Multiple methods of structure-based modulator  
design are known to those in the art. Kuntz et al.,  
20 1982, *J. Mol. Biol.* 162: 269; Kuntz et al., 1994,  
*Acc. Chem. Res.* 27: 117; Meng et al., 1992, *J. Compt.*  
*Chem.* 13: 505; Bohm, 1994, *J. Comp. Aided Molec. Design*  
8: 623.

A computer program widely utilized by those skilled  
25 in the art of rational modulator design is DOCK from the  
University of California in San Francisco. The general  
methods utilized by this computer program and programs  
like it are described in three applications below. More  
detailed information regarding some of these techniques  
30 can be found in the Molecular Simulations User Guide,  
1995.



A typical computer program used for this purpose can comprise the following steps:

- (a) remove the existing compound from the protein;
- (b) dock the structure of another compound into the active-site using the computer program (such as DOCK) or by interactively moving the compound into the active-site;
- (c) characterize the space between the compound and the active-site atoms;
- (d) search libraries for molecular fragments which (i) can fit into the empty space between the compound and the active-site, and (ii) can be linked to the compound; and
- (e) link the fragments found above to the compound and evaluate the new modified compound.

Part (c) refers to characterizing the geometry and the complementary interactions formed between the atoms of the active-site and the compounds. A favorable geometric fit is attained when a significant surface area is shared between the compound and active-site atoms without forming unfavorable steric interactions.

One skilled in the art would note that the method can be performed by skipping parts (d) and (e) and screening a data base of many compounds.

Structure-based design and identification of modulators of PTK function can be used in conjunction with assay screening. As large computer data base of compounds (around 10,000 compounds) can be searched in a matter of hours, the computer based method can narrow the compounds tested as potential modulators of PTK function in cellular assays.

The above descriptions of structure-based modulator design are not all encompassing and other methods are reported in the literature:

5 (1) CAVEAT: Bartlett et al., 1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M.; Ley, S.V.; Campbell, M.M. eds.; Royal Society of Chemistry: Cambridge, ppl82-196.

(2) FLOG: Miller et al., 1994, *J. Comp. Aided Molec. Design* 8:153.

10 (3) PRO Modulator: Clark et al., 1995, *J. Comp. Aided Molec. Design* 9:13.

(4) MCSS: Miranker and Karplus, 1991, *Proteins: Structure, Function, and Genetics* 11:29.

15 (5) AUTODOCK: Goodsell and Olson, 1990, *Proteins: Structure, Function, and Genetics* 8:195.

(6) GRID: Goodford, 1985, *J. Med. Chem.* 28:849.

Design by Modifying Compounds in Complex with PTKs

20 Another way of identifying compounds as potential modulators is to modify an existing modulator in the polypeptide active-site. For example, the computer representation of modulators can be modified within the computer representation of a PTK active-site. Detailed instructions for this technique can be found in the  
25 Molecular Simulations User Manual, 1995 in LUDI. The computer representation of the modulator is modified by the deletion of a chemical group or groups or by the addition of a chemical group or groups.

30 Upon each modification to the compound, the atoms of the modified compound and active-site can be shifted in conformation and the distance between the modulator

and the active-site atoms may be scored along with any complimentary interactions formed between the two molecules. Scoring can be complete when a favorable geometric fit and favorable complementary interactions are attained. Compounds that have favorable scores are potential modulators of PTK function.

Design by Modifying the Structure of Compounds that Bind PTKs

10           A third method of structure-based modulator design is to screen compounds designed by a modulator building or modulator searching computer program. Examples of these types of programs can be found in the Molecular Simulations Package, Catalyst. Descriptions for using this program are documented in the Molecular Simulations User Guide (1995). Other computer programs used in this application are ISIS/HOST, ISIS/BASE, ISIS/DRAW) from Molecular Designs Limited and UNITY from Tripos Associates.

20           These programs can be operated on the structure of a compound that has been removed from the active-site of the three dimensional structure of a compound-PTK complex. Operating the program on such a compound is preferable since it is in a biologically active conformation.

25           A modulator construction computer program is a computer program that may be used to replace computer representations of chemical groups in a compound complexed with a PTK with groups from a computer data base. A modulator searching computer program is a computer program that may be used to search computer

representations of compounds from a computer data base that have similar three dimensional structures and similar chemical groups as compound bound to a PTK.

A typical program can operate by using the following general steps:

- (a) map the compounds by chemical features such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites;
- (b) add geometric constraints to the mapped features; and
- (c) search data bases with the model generated in (b).

Those skilled in the art recognize that for indolinones, the important chemical features include, but are not limited to, a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Those skilled in the art also recognize that not all of the possible chemical features of the compound need be present in the model of (b). One can use any subset of the model to generate different models for data base searches.

#### IX. Organic Synthetic Techniques

The versatility of computer-based modulator design and identification lies in the diversity of structures screened by the computer programs. The computer programs can search data bases that contain 200,000 molecules and can modify modulators already complexed with the enzyme with a wide variety of chemical

functional groups. A consequence of this chemical diversity is that a potential modulator of PTK function may take a chemical form that is not predictable. A wide array of organic synthetic techniques exist in the art to meet the challenge of constructing these potential modulators of PTK function. Many of these organic synthetic methods are described in detail in standard reference sources utilized by those skilled in the art. One example of such a reference is March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill. Thus, the techniques required to synthesize a potential modulator of PTK function identified by computer-based methods are readily available to those skilled in the art of organic chemical synthesis.

X. Cellular Assays Measuring the Effect of a PTK Modulator in Signal Transduction Pathways

Cellular assays can be used to test the activity of a potential modulator of PTK function as well as diagnose a disease associated with inappropriate PTK activity. A potential modulator of PTK function can be tested for activity *in vitro* by assays that measure the effect of a potential modulator on the autophosphorylation of a particular PTK over-expressed in a cell line. Thus, a modulator that acts as a potent inhibitor of the catalytic domain corresponding to a PTK would decrease the amount of autophosphorylation catalyzed by that PTK. Potential modulators could also be tested for activity in cell growth assays *in vitro* as well as in animal model assays *in vivo*.

In vivo assays are also useful for testing the bioactivity of a potential modulator designed by the methods of the invention.

Materials, methods, and experimental data for these assays are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

XI. Administration of Modulators of PTK Function as Therapeutics for Disease

Methods of administering compounds to organisms as therapeutics for disease are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

EXAMPLES

The examples below are non-limiting and are merely representative of various aspects and features of the present invention. The examples provide illustrative methods for obtaining crystalline forms of protein kinase polypeptides, methods for determining three dimensional structures of these protein kinase polypeptides, and methods for identifying modulators of protein kinases using the three dimensional structures of the protein kinases.

EXAMPLE 1: X-ray Crystallographic Structure  
Determination of FGFR1

Polypeptide Synthesis and Isolation

5 A recombinant baculovirus was engineered to encode residues 456-765 of human FGFR1. A cleavable N-terminal histidine tag was incorporated to aid in protein purification. Three amino acid substitutions were introduced: Cys-488 to Ala, Cys-584 to Ser and Leu-457  
10 to Val. The two cysteine substitutions were made to prevent the formation of disulfide-linked oligomers, which occurs for the native protein. The substitution Leu-457 to Val introduced a *Nco*I cloning site near Met-456. The codon for Tyr-766 (TAC) was changed to a stop  
15 codon (TAG) and a *Hind*III-cloning site was generated following this stop codon. These substitutions were introduced into the full length human cDNA of FGFR1 in m13MPI9 by site-directed mutagenesis according to the manufacturer's protocol (Amersham).

20 The resulting construct was digested with *Nco*I and *Hind*III and was ligated into appropriately digested pBlueBac HistagB (Invitrogen). Transfection of insect cells (Sf9) was performed with the BaculoGold transfection system according to the manufacturer's  
25 protocol (Pharmingen). Following identification of positive plaques, the recombinant baculovirus was amplified to high titer ( $5 \times 10^7$  virus particles/ml). Sf9 cells were grown in 175-cm<sup>2</sup> flasks to a density of  $2-3 \times 10^7$  per flask and infected with recombinant baculovirus  
30 with a multiplicity of infection (MOI) of 10.

After 48 hr, cells were harvested by centrifugation

at 3,000g for 35 min at 4°C and then lysed in 25 mM  
HEPES (pH 7.5), 150 mM NaCl, 10% glycerol, 1.5 mM MgCl<sub>2</sub>,  
1 % Triton X-100, 10 µg/ml aprotonin, 10 µg/ml  
leupeptin, and 1 mM phenylmethylsulfonyl fluoride  
(PMSF). Lysates were centrifuged in a Sorval RC 5C  
(Dupont) for 1 hr at 4°C at 40,000g followed by  
ultracentrifugation in an XL-80 (Beckman) at 100,000g  
for 1 hr. After centrifugation, the clarified lysate  
was passed over a Ni<sup>2+</sup>-chelating column (Pharmacia), and  
the bound histidine-tagged fusion protein was eluted  
with 100 mM imidazole (pH 7.5). Pooled fractions were  
loaded onto a Mono Q anion exchange column (Pharmacia)  
and eluted with a NaCl gradient from 0 to 500 mM.

The fractions containing the fusion protein were  
concentrated in a Centricon-30 (Amicon), and the  
histidine tag was removed by overnight digestion with  
enterokinase (Biozyme) at 20°C. The digestion was  
terminated by the addition of aprotonin, leupeptin,  
PMSF, TPCK, and bovine pancreatic trypsin inhibitor  
(BPTI). The cleaved kinase domain was then separated  
from the histidine tag on a Superose 12 size-exclusion  
column (Pharmacia). The eluted kinase domain was  
further purified on a Mono Q column. The purified  
kinase domain was analyzed by N-terminal sequencing and  
mass spectrometry. Five amino acids (SAAGT) remained  
from the histidine tag. The predicted molecular mass  
was confirmed by mass spectrometry.

#### Crystal Growth

Purified FGFR1 was concentrated to 20-50 mg/ml and  
exchanged into 10 mM Tris-HCl (pH 8.0), 10 mM NaCl, and



2 mM DTT using a Centricon-30. Crystals were grown at 4°C by vapor diffusion in hanging drops containing 2.0 µl of 10 mg/ml protein solution and 2.0 µl of reservoir solution: 16% polyethylene glycol (PEG) 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol, and 100 mM bis-Tris (pH 6.5).

Crystals of native FGFR1 were soaked in 500 ml stabilizing solution [25% PEG 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 0.1 M Bis-Tris (pH 6.5), 5% ethylene glycol] containing 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone (1-5 mM) or 3-[4-(4-formylpiperazine-1-yl)-benzylidenyl]-2-indolinone (1 mM) at 4°C for 24 to 48 hours. The final soaking concentration of DMSO was between 1 to 5%. The crystals cracked at higher concentrations of DMSO.

Co-crystals of FGFR1 with the inhibitors could also be obtained by vapor diffusion in hanging drops containing 2.0 µl of 10 mg/ml protein solution and 2.0 µl of reservoir solution containing 1 mM 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone and 3-[4-(4-formylpiperazine-1-yl)-benzylidenyl]-2-indolinone.

Co-crystals of FGFR1 complexed with AMP-PCP were obtained as described for the creation of native crystals, except that the protein solution additionally contained 10 mM AMP-PCP and 20 mM MgCl<sub>2</sub>.

#### Preparation Of Heavy Atom Derivative Crystals

Heavy atom derivative crystals were obtained by soaking FGFR1 native crystals (C2-A form) in a solution containing ethylmercurithiosalicylic acid (thimerosal),

KAu(CN)<sub>2</sub> or 4-chloromercuribenzoic acid, as provided in Table 1, *infra*, and containing 25% PEG 10000, 0.3M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol or glycerol, and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (Synchrotron) or in a dry nitrogen stream at -175°C (rotating anode).

#### Data Collection and Structure Determination

For native crystals and crystals comprising the nucleotide analog AMP-PCP, data were collected either on a Rigaku RU-200 rotating anode operated at 50 kV and 100 mA (Cu K $\alpha$ ) and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector, or at beamline X-4A at the National Synchrotron Light Source, Brookhaven National Laboratory. Synchrotron data ( $\lambda=1.07\text{\AA}$ ) were collected on Fuji image plates and read with a Fuji scanner. One cryo-cooled crystal was used for each of the data sets. To obtain cryo-cooled crystals, crystals were soaked in a cryo-protectant solution containing 25% PEG 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol or glycerol and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (synchrotron data) or in a dry nitrogen stream at -175°C (rotating anode data). All data were processed using DENZO and SCALEPACK. Otwinowski, 1993, "Oscillation data reduction program," Proceedings of the CCP4 Study Weekend, Sawyer et al., eds. (Daresbury, United Kingdom: SERC Daresbury Laboratory), 56-62.

For native crystals and crystals comprising the nucleotide analog AMP-PCP, a molecular replacement solution was found initially for the C2-B crystal form

using an IRK search model that consisted of polyalanine with the common side chains for residues 993-1263 (FGFR1 residues 475-754), excluding residues 1094-1105 (kinase insert) and 1153-1170 (activation loop). With AMORE

5 (Navaza, 1994, *AmoRe: an automated package for molecular replacement*," *Acta Crystallogr. A*50: 157-163), using 80% of the structure factor amplitudes between 15.0 and 3.5 Å, one of the two molecules in the asymmetric unit was located. The correlation coefficient (c.c.) for the  
10 correct 1-molecule solution was 0.23 (versus 0.20 for the highest incorrect solution). This molecule was rigid body-refined in X-PLOR (Brünger, 1992, X-PLOR (Version 3.1) Manual (New Haven, Connecticut: The Howard Hughes Medical Institute and Department of Molecular  
15 Biophysics and Biochemistry, Yale University)), first as one rigid body unit, then as two units each comprising a lobe of the kinase. Rigid body refinement (12.0-3.5 Å,  $F > 3\sigma$ ) resulted in a relative rotation of the two lobes of  $\sim 10^\circ$  and an increase of the c.c. from 0.20 to 0.25.  
20 The rigid body-refined molecule was then used as a new search model in AMORE, and this time both molecules in the asymmetric unit were located. The c.c. for the correct 2-molecule solution was 0.35 (versus 0.27 for the highest incorrect solution).

25 Multiple cycles of model building and refinement against 6.0-2.4 Å data resulted in the addition to the model of many of the side chains and some of the missing polypeptide chain. Model building was performed using TOM/FRODO (Jones, 1985, "Diffraction methods for  
30 biological macromolecules. Interactive computer graphics: FRODO," *Methods in Enzymology* 115: 157-171)

and conjugate-gradient minimization and simulated annealing were performed using X-PLOR. Brünger, *supra*. At this stage, the R-value was 30% (free R-value of 36%). To help expedite model building and refinement, experimental phases were obtained. Because crystals grown in the presence of ethylene glycol were easier to manipulate than those grown in glycerol, several heavy-atom derivative data sets were collected from C2-A crystals that had been soaked in various heavy atom solutions. The C2-B structure was subsequently refined against 6.0-2.4 Å data to an R-value of 23.8% (free R-value of 30.4%) with r.m.s.d. values of 0.008 Å for bond distances and 1.4° for bond angles.

Molecular replacement was used to locate the two FGFR1 molecules (designated FLGK-A and FLGK-B) in the asymmetric unit of the C2-A crystal form. Using AMORE with 80% of structure factor amplitudes between 15.0 and 3.5 Å and the C2-B model, the c.c. for the correct 2-molecule solution was 0.62 (versus 0.35 for the highest incorrect solution). Heavy atom positions were determined from difference Fourier maps using the calculated phases from the partial model. Refinement of heavy atom parameters and phase determination were performed with MLPHARE (Otwinowski, 1991, "Maximum likelihood refinement of heavy atom parameters," *Isomorphous replacement and anomalous scattering*, Evans and Leslie eds. (Daresbury, United Kingdom: SERC Daresbury Laboratory), 56-62)). An initial molecular isomorphous replacement (MIR)-phased electron density map was calculated with data between 2.0. and 2.8 Å resolution. This map was improved by solvent

flattening, histogram matching, and non-crystallographic symmetry (NCS) averaging using DM (Cowtan, 1994, "Protein Crystallography," *CCP4 and ESF-EACBM Newsletter (joint)* 31: 34-38).

5           Refinement of the C2-A FGFR1 structure against 6.0-2.0 Å data proceeded by conjugate-gradient minimization and simulated annealing using X-PLOR. Tight NCS restraints were imposed until data to 2.0 Å resolution were included in the refinement, at which point the  
10           restraints were lifted. An overall anisotropic B-value was calculated using X-PLOR and applied to the observed structure factors, reducing the R-value by ~3%. Water molecules whose B-values refined to  $\geq 70$  Å<sup>2</sup> were omitted from the subsequent refinement round. The average B-  
15           value is 37.5 Å<sup>2</sup> for all protein atoms, 35.4 Å<sup>2</sup> for protein atoms in FLGK-A, 39.7 Å<sup>2</sup> for protein atoms in FLGK-B, and 40.2 Å<sup>2</sup> for water molecules. The side chains for Cys-603 in FLGK-A and FLGK-B and for Met-534 in FLGK-B have been modeled in two different conformations.  
20           Residues that are not included in the atomic model due to poor supporting electron density are for FLGK-A: 456-463, 486-490, 501-504, 580-591, 763-765; and for FLG-B: 456-460, 501-504, 578-593, 646-651, 657-659, 762-765.

          The positions of the two AMP-PCP molecules (one per  
25           FGFR1 molecule) were easily identified in  $2F_{\text{obs(co-complex)}} - F_{\text{calc(FGFR1)}}$  difference Fourier maps. The AMP-PCP molecule bound to FLGK-B is less tightly bound and has been modeled with an occupancy of 0.5.

          Table A summarizes the X-ray crystallography data  
30           sets of FGFR1 derivative crystals that were used to determine the structures of crystalline FGFR1 and

crystalline FGFR1:AMP-PCP co-complex of the invention.

TABLE 5

Data Collection and MIR Phasing Summary						
	Native	AMP-PCP	Thi-1 <sup>a</sup>	Thi-2 <sup>a</sup>	PCMB <sup>a</sup>	KAu(CN) <sub>2</sub>
X-ray source	X-4A	RU-200	RU-200	RU-200	RU-200	RU-200
Resolution limit (Å)	2.0	2.3	2.6	2.8	2.8	2.8
Number of sites	—	—	4	7	2	2
Conc. (mM)/time (h)	—	—	0.1/24	0.1/48	0.2/2	5.0/72
R <sub>sym</sub> <sup>b</sup> (%)	4.8(19.7) <sup>c</sup>	4.5(23.3) <sup>c</sup>	5.5	9.8	6.8	6.8
Total observations	122569	91324	55456	59488	67988	45303
Unique reflections	50771	31997	42820 <sup>d</sup>	35538 <sup>d</sup>	18619	18202
Completeness (%)	97.3(96.3) <sup>c</sup>	95.5(93.7) <sup>c</sup>	95.0	96.7	98.0	97.7
Signal (%I>3σ)	80.7(50.3) <sup>c</sup>	79.6(51.7) <sup>c</sup>	69.8	66.8	84.7	77.6
R <sub>iso</sub> <sup>e</sup> (%)	—	—	17.1	31.2	15.4	15.2
Phasing power <sup>f</sup>	—	—	1.8	2.0	1.0	0.9
R <sub>cullis</sub> <sup>g</sup> (%)	—	—	0.55	0.50	0.81	0.84
Overall FOM <sup>h</sup>				0.60		

<sup>a</sup>Thi-1, Thi-2; ethylmercurithiosalicylic acid (thimerosal); PCMB: 4-chloromercuribenzoic acid.

<sup>b</sup>R<sub>sym</sub> = 100 × Σ<sub>i</sub> |I<sub>i</sub>(h) - <I(h)>| / Σ<sub>i</sub> I<sub>i</sub>(h)

<sup>c</sup>Value in parentheses is for the highest resolution shell.

<sup>d</sup>I(+h) and I(-h) processed as independent reflections. Anomalous scattering contributions were included.

<sup>e</sup>R<sub>iso</sub> = 100 × Σ<sub>h</sub> ||F<sub>p</sub>(h) ± F<sub>p</sub>(h)| - |F<sub>PH</sub>(h)|| / Σ<sub>h</sub> |F<sub>p</sub>(h)|, where F<sub>p</sub> and F<sub>PH</sub> are the native and derivative structure factors, respectively.

<sup>f</sup>Phasing power: r.m.s. heavy atom structure factor / r.m.s. lack of closure (for acentric reflections from 20.0 to 2.8 Å).

<sup>g</sup>R<sub>cullis</sub> = 100 × Σ<sub>h</sub> ||F<sub>PH</sub>(h) - F<sub>H(calc)</sub>(h)| / Σ<sub>h</sub> |F<sub>PH</sub>(h) ± F<sub>p</sub>(h)| (for centric reflections from 20.0 to 2.8 Å).

<sup>h</sup>Figure of merit: ∫ P(φ)exp(iφ)dφ / ∫ P(φ)d(φ), where P is the probability distribution of the phase angle φ.

For crystals comprising FGFR1 and compounds 1 and 2, data were collected on a Rigaku RU-200 rotating anode (Cu K $\alpha$ ) operating at 50 kV and 100 mA and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector. One cryo-cooled crystal was used for each of the data sets. Crystals were soaked in a cryo-protectant [25% PEG 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol, 100 mM bis-Tris (pH 6.5), and 1 mM: 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone (hereafter referred to as compound 1) or 3-[4-(4-formylpiperazine-1-yl)-benzylidenyl]-2-indolinone (hereafter referred to as compound 2) and flash-cooled in a dry nitrogen stream at -175°C. Data were processed using DENZO and SCALEPACK. Otwinowski, 1993; *Proceedings of the CCP4 Study Weekend* (Daresbury, United Kingdom: SERC Daresbury Laboratory) pp 56-62.

A summary of the data collection parameters are included in the following Table 6:

TABLE 6

	Resolution limit (Å)	Observations (N)	Completeness (%)	Redundancy	R <sub>sym</sub> <sup>a</sup> (%)	Signal (I > $\sigma$ I)
compound 1	2.5	93535	97.6 (96.1)	2.7	6.8 (23.0)	11.8
compound 2	2.4	94093	99.1 (97.9)	3.3	6.3 (32.2)	11.4

compound 1 structure: 550 residues, 252 water molecules, 2 compound 1 molecules (4589 atoms)

compound 2 structure: 550 residues, 248 water molecules, 2 compound 2 molecules (4646 atoms)

### Structure Analyses

Atomic superpositions were performed with TOSS

(Hendrickson, 1979). Per residue solvent accessible surface calculations were done with X-PLOR. The surface area buried in a dimer interface was calculated with GRASP (Nicholls et al., 1991) using a probe radius of 1.4 Å. The stereochemical quality of the atomic model was monitored using PROCHECK (Laskowski et al., 1993, PROCHECK: a computer program to check the stereochemical quality of protein structures," *J. Appl. Cryst.* 26: 283-291). As defined in PROCHECK, 93% of the residues in the model have main-chain torsion angles in the most favored Ramachandran regions. There are no residues in disallowed regions, and three residues in generously allowed regions: Arg-622 in FLGK-A and FLGK-B and Arg-554 in FLGK-A. The overall G-factor score is 0.42.

Table 7 summarizes the X-ray crystallography refinement parameters of the structures of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex of the invention. Table 8 summarizes the X-ray crystallography refinement parameters for the FGFR1/compound complexes.

TABLE 7

Refinement Parameters						
FGFR1: 550 residues, 252 water molecules (4589 atoms)						
FGFR1:AMP-PCP: 550 residues, 238 water molecules, 2 AMP-PCP molecules (4638 atoms)						
Model	d-spacings (Å)	Reflections (N)	R-value <sup>a</sup> (%)	bonds (Å)	angles (°)	B-values <sup>b</sup> (Å <sup>2</sup> )
FGFR1:	6.0-2.0	42548	21.3 (26.2) <sup>c</sup>	0.008	1.3	1.6
FGFR1:AMP-PCP:	6.0-2.3	26729	20.1 (27.5) <sup>c</sup>	0.009	1.4	1.7

<sup>a</sup>R-value =  $100 \times \sum_h ||F_{obs}(h)| - |F_{calc}(h)|| / \sum_h |F_{obs}(h)|$  for reflections with  $F_{obs} > 2\sigma$ .



<sup>b</sup>For bonded protein atoms.

<sup>c</sup>Value in parentheses is the free R-value (Brünger, 1993) determined from 5% of the data.

TABLE 8

Model	d-spacings (Å)	Reflec- tions	R- value <sup>i</sup> (N)	bonds (Å)	angles (°)	B- values <sup>j</sup> (Å <sup>2</sup> )
compound 1	6.0–2.4	42548	19.7 (27.0) <sup>k</sup>	0.008	1.3	1.6
compound 2	6.0–2.5	26729	20.0 (28.0) <sup>k</sup>	0.008	1.4	1.7

$$^a R_{\text{sym}} = 100 \times S_h S_l |I_i(h) - I(h)^o| / S_h S_l I_i(h)$$

<sup>c</sup>Value in parentheses is for the highest resolution shell.

<sup>i</sup>R-value =  $100 \times S_h \sum |F_o(h) - F_c(h)| / S_h \sum |F_o(h)|$ , where  $F_o$  and  $F_c$  are the observed and calculated structure factors, respectively ( $F_o > 2s$ ).

<sup>j</sup>For bonded protein atoms.

<sup>k</sup>Value in parentheses is the free R-value determined from 5% of the data.

### Atomic Structural Coordinates

Tables 1 and 2 provide the atomic structural coordinates of unphosphorylated FGFR1 and unphosphorylated FGFR1:AMP-PCP co-complex, respectively. In the Tables, coordinates for both of the FGFR1 molecules of the dimer comprising the asymmetric unit are provided. The amino acid residue numbers coincide with those used in FIG. 3. In the first FGFR1 molecule of the dimer the residue number is preceded by a 1, i.e., residue number 464 of the first FGFR1 molecule of the dimer is denoted by "1464". Tables 3 and 4 provide the atomic structural coordinates of FGFR1 in complex with indolinone compounds found to inhibit FGFR1 function.

The following abbreviations are used in the Tables:

"Atom Type" refers to the element whose coordinates are provided. The first letter in the column defines the element.

5        "A.A." refers to amino acid.

      "X, Y and Z" provide the Cartesian coordinates of the element.

      "B" is a thermal factor that measures movement of the atom around its atomic center.

10       "OCC" refers to occupancy, and represents the percentage of time the atom type occupies the particular coordinate. OCC values range from 0 to 1, with 1 being 100%.

      "PRT1" or "PRT2" relate to occupancy, with PRT1  
15       designating the coordinates of the atom when in the first conformation and PRT2 designating the coordinates of the atom when in the second or alternate conformation.

      Structural coordinates for FGFR1 may be modified by  
20       mathematical manipulation. Such manipulations include, but are not limited to, crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or  
      subtractions to sets of the raw structure coordinates,  
25       inversion of the raw structure coordinates and any combination of the above.

      In addition, the structural coordinates can be slightly modified and still render nearly identical  
      three dimensional structures. Therefore, a measure of a  
30       unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural

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in 100mM sodium bicarbonate (pH 9.6) buffer overnight at 4°C.

2. Wash the column once with PBS.
3. Block the excess sites on the column with 2 M glycine for 2 hours at 4°C.
4. Wash the column with PBS.
5. Incubate the column with Rabbit anti-Flk-1D production bleed for 2 hours at 4°C.
6. Wash the column with PBS.
7. Elute antiserum with 100 mM Citric Acid, pH3.0 and neutralize the eluate immediately with 2 M Tris, pH 9.0.
8. Dialyze the eluate against PBS overnight at 4°C with 3 changes of buffer (sample to buffer ratio is 1:100).
9. Adjust the dialyzed antiserum to 5% glycerol and store at -80°C in small aliquotes.

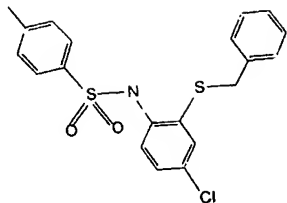
The Flk-1 ELISA can include a 2,2-azino-bis(3-ethylbenz-thiazoline-6-sulfonic acid (ABTS) solution, which can comprise 100mM citric acid (anhydrous), 250 mM Na<sub>2</sub>HPO<sub>4</sub> (pH 4.0), 0.5 mg/ml ABTS (Sigma catalog no. A-1888). The solution is most appropriately stored in dark at 4°C until ready for use.

The FLK-1 specific antibodies can also be purchased from Santa Cruz Biotechnology (Catalog No. SC-504).

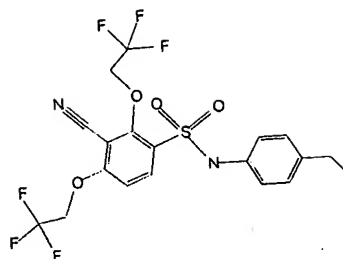
Four of the forty compounds identified as potential modulators of PTK function were potent modulators of FLK function. These molecules have the following structures:

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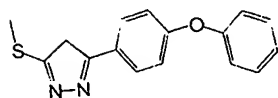
1



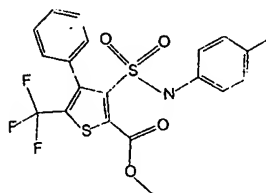
2



3



4



The modulators inhibit the FLK protein kinase with the following  $IC_{50}$  values:

TABLE 9

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Compound	FLK kinase $IC_{50}$ ( $\mu M$ ) compounds tested at 100 $\mu M$	FLK kinase $IC_{50}$ ( $\mu M$ ) compounds tested at 20 $\mu M$	EGFR $IC_{50}$ ( $\mu M$ )	IGF-1R $IC_{50}$ ( $\mu M$ )
1	14.8	14	>100	>100
2	15.7	10.6	>100	>100
3	21.4	16.6	68	30.9
4	22.9	16.4	>100	>100

10

The invention illustratively described herein may be practiced in the absence of any element or elements, limitation or limitations which is not specifically disclosed herein. The terms and expressions which have

been employed are used as terms of description and not of limitation, and there is no intention that in the use of such terms and expressions of excluding any equivalents of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention claimed. Thus, it should be understood that although the present invention has been specifically disclosed by preferred embodiments and optional features, modification and variation of the concepts herein disclosed may be resorted to by those skilled in the art, and that such modifications and variations are considered to be within the scope of this invention as defined by the appended claims.

Those references not previously incorporated herein by reference, including both patent and non-patent references, are expressly incorporated herein by reference for all purposes. Other embodiments are within the following claims.

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SEQUENCE LISTING

## (1) GENERAL INFORMATION:

- (i) APPLICANT: SUGEN, INCORPORATED  
351 Galveston Drive  
Redwood City, CA 94063
- (ii) TITLE OF INVENTION: CRYSTAL STRUCTURES OF A  
PROTEIN TYROSINE KINASE
- (iii) NUMBER OF SEQUENCES: 5
- (iv) CORRESPONDENCE ADDRESS:
- |                |                       |
|----------------|-----------------------|
| (A) ADDRESSEE: | Lyon & Lyon           |
| (B) STREET:    | 633 West Fifth Street |
|                | Suite 4700            |
| (C) CITY:      | Los Angeles           |
| (D) STATE:     | California            |
| (E) COUNTRY:   | U.S.A.                |
| (F) ZIP:       | 90071-2066            |
- (v) COMPUTER READABLE FORM:
- |                       |                                   |
|-----------------------|-----------------------------------|
| (A) MEDIUM TYPE:      | 3.5" Diskette, 1.44 Mb<br>storage |
| (B) COMPUTER:         | IBM Compatible                    |
| (C) OPERATING SYSTEM: | IBM P.C. DOS 5.0                  |
| (D) SOFTWARE:         | FastSEQ for Windows 2.0           |
- (vi) CURRENT APPLICATION DATA:
- |                         |                |
|-------------------------|----------------|
| (A) APPLICATION NUMBER: | To Be Assigned |
| (B) FILING DATE:        | Herewith       |
| (C) CLASSIFICATION:     |                |
- (vii) PRIOR APPLICATION DATA:
- |                         |  |
|-------------------------|--|
| (A) APPLICATION NUMBER: |  |
| (B) FILING DATE:        |  |

110

## (viii) ATTORNEY/AGENT INFORMATION:

(A) NAME: Warburg, Richard J.  
 (B) REGISTRATION NUMBER: 32,327  
 (C) REFERENCE/DOCKET NUMBER: 227/088-PCT

## (ix) TELECOMMUNICATION INFORMATION:

(A) TELEPHONE: (213) 489-1600  
 (B) TELEFAX: (213) 955-0440  
 (C) TELEX: 67-3510

## (2) INFORMATION FOR SEQ ID NO:1:

## (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 310 amino acids  
 (B) TYPE: amino acid  
 (C) STRANDEDNESS: single  
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

## (xi) SEQUENCE DESCRIPTION: SEQ ID NO:1:

Met Leu Ala Gly Val Ser Glu Tyr Glu Leu Pro Glu Asp Pro Arg Trp  
 1 5 10 15  
 Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys Pro Leu Gly Glu Gly  
 20 25 30  
 Cys Phe Gly Gln Val Val Leu Ala Glu Ala Ile Gly Leu Asp Lys Asp  
 35 40 45  
 Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys Met Leu Lys Ser Asp  
 50 55 60  
 Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser Glu Met Glu Met Met  
 65 70 75 80  
 Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn Leu Leu Gly Ala Cys  
 85 90 95  
 Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu Tyr Ala Ser Lys Gly  
 100 105 110  
 Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro Pro Gly Leu Glu Tyr  
 115 120 125  
 Cys Tyr Asn Pro Ser His Asn Pro Glu Glu Gln Leu Ser Ser Lys Asp  
 130 135 140



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Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly Met Glu Tyr Leu Ala  
 145 150 155 160  
 Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala Arg Asn Val Leu Val  
 165 170 175  
 Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe Gly Leu Ala Arg Asp  
 180 185 190  
 Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr Asn Gly Arg Leu Pro  
 195 200 205  
 Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp Arg Ile Tyr Thr His  
 210 215 220  
 Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu Trp Glu Ile Phe Thr  
 225 230 235 240  
 Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val Glu Glu Leu Phe Lys  
 245 250 255  
 Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro Ser Asn Cys Thr Asn  
 260 265 270  
 Glu Leu Tyr Met Met Met Arg Asp Cys Trp His Ala Val Pro Ser Gln  
 275 280 285  
 Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu Asp Arg Ile Val Ala  
 290 295 300  
 Leu Thr Ser Asn Gln Glu  
 305 310

## (2) INFORMATION FOR SEQ ID NO:2:

## (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 315 amino acids  
 (B) TYPE: amino acid  
 (C) STRANDEDNESS: single  
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:2:

Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu Tyr Glu Leu Pro  
 1 5 10 15  
 Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys  
 20 25 30

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Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Val Leu Ala Glu Ala Ile  
 35 40 45

Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys  
 50 55 60

Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser  
 65 70 75 80

Glu Met Glu Met Met Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn  
 85 90 95

Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu  
 100 105 110

Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro  
 115 120 125

Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn Pro Glu Glu Gln  
 130 135 140

Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly  
 145 150 155 160

Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala  
 165 170 175

Arg Asn Val Leu Val Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe  
 180 185 190

Gly Leu Ala Arg Asp Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr  
 195 200 205

Asn Gly Arg Leu Pro Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp  
 210 215 220

Arg Ile Tyr Thr His Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu  
 225 230 235 240

Trp Glu Ile Phe Thr Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val  
 245 250 255

Glu Glu Leu Phe Lys Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro  
 260 265 270

Ser Asn Cys Thr Asn Glu Leu Tyr Met Met Met Arg Asp Cys Trp His  
 275 280 285

Ala Val Pro Ser Gln Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu  
 290 295 300

Asp Arg Ile Val Ala Leu Thr Ser Asn Gln Glu  
 305 310 315

WO 98/07835

113

## (2) INFORMATION FOR SEQ ID NO:3:

## (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 351 amino acids  
 (B) TYPE: amino acid  
 (C) STRANDEDNESS: single  
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

## (xi) SEQUENCE DESCRIPTION: SEQ ID NO:3:

Met Arg Gly Ser His His His His His His Gly Met Ala Ser Met Thr  
 1 5 10 15  
 Gly Gly Gln Gln Met Gly Arg Asp Leu Tyr Asp Asp Asp Asp Lys Asp  
 20 25 30  
 Pro Ser Ser Arg Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu  
 35 40 45  
 Tyr Glu Leu Pro Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu  
 50 55 60  
 Val Leu Gly Lys Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Val Leu  
 65 70 75 80  
 Ala Glu Ala Ile Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys  
 85 90 95  
 Val Ala Val Lys Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser  
 100 105 110  
 Asp Leu Ile Ser Glu Met Glu Met Met Lys Met Ile Gly Lys His Lys  
 115 120 125  
 Asn Ile Ile Asn Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr  
 130 135 140  
 Val Ile Val Glu Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln  
 145 150 155 160  
 Ala Arg Arg Pro Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn  
 165 170 175  
 Pro Glu Glu Gln Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln  
 180 185 190  
 Val Ala Arg Gly Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg  
 195 200 205

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Asp Leu Ala Ala Arg Asn Val Leu Val Thr Glu Asp Asn Val Met Lys  
 210 215 220  
 Ile Ala Asp Phe Gly Leu Ala Arg Asp Ile His His Ile Asp Tyr Tyr  
 225 230 235 240  
 Lys Lys Thr Thr Asn Gly Arg Leu Pro Val Lys Trp Met Ala Pro Glu  
 245 250 255  
 Ala Leu Phe Asp Arg Ile Tyr Thr His Gln Ser Asp Val Trp Ser Phe  
 260 265 270  
 Gly Val Leu Leu Trp Glu Ile Phe Thr Leu Gly Gly Ser Pro Tyr Pro  
 275 280 285  
 Gly Val Pro Val Glu Glu Leu Phe Lys Leu Leu Lys Glu Gly His Arg  
 290 295 300  
 Met Asp Lys Pro Ser Asn Cys Thr Asn Glu Leu Tyr Met Met Met Arg  
 305 310 315 320  
 Asp Cys Trp His Ala Val Pro Ser Gln Arg Pro Thr Phe Lys Gln Leu  
 325 330 335  
 Val Glu Asp Leu Asp Arg Ile Val Ala Leu Thr Ser Asn Gln Glu  
 340 345 350

## (2) INFORMATION FOR SEQ ID NO:4:

## (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 933 base pairs  
 (B) TYPE: nucleic acid  
 (C) STRANDEDNESS: double  
 (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: cDNA to mRNA

## (xi) SEQUENCE DESCRIPTION: SEQ ID NO:4:

ATGCTAGCAG GGGTCTCTGA GTATGAGCTT CCCGAAGACC CTCGCTGGGA GCTGCCTCGG 60  
 GACAGACTGG TCTTAGGCAA ACCCCTGGGA GAGGGCTGCT TTGGGCAGGT GGTGTTGGCA 120  
 GAGGCTATCG GGCTGGACAA GGACAAACCC AACCGTGTGA CCAAAGTGGC TGTGAAGATG 180  
 TTGAAGTCGG ACGCAACAGA GAAAGACTTG TCAGACCTGA TCTCAGAAAT GGAGATGATG 240  
 AAGATGATCG GGAAGCATAA GAATATCATC AACCTGCTGG GGGCCTGCAC GCAGGATGGT 300  
 CCCTTGATG TCATCGTGGA GTATGCCTCC AAGGGCAACC TGCGGGAGTA CCTGCAGGCC 360  
 CGGAGGCCCC CAGGGCTGGA ATACTGCTAC AACCCAGCC ACAACCCAGA GGAGCAGCTC 420

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TCCTCCAAGG ACCTGGTGTC CTGCGCCTAC CAGGTGGCCC GAGGCATGGA GTATCTGGCC 480  
TCCAAGAAGT GCATACACCG AGACCTGGCA GCCAGGAATG TCCTGGTGAC AGAGGACAAT 540  
GTGATGAAGA TAGCAGACTT TGGCCTCGCA CGGGACATTC ACCACATCGA CTACTATAAA 600  
AAGACAACCA ACGGCCGACT GCCTGTGAAG TGGATGGCAC CCGAGGCATT ATTTGACCGG 660  
ATCTACACCC ACCAGAGTGA TGTGTGGTCT TTCGGGGTGC TCCTGTGGGA GATCTTCACT 720  
CTGGGCGGCT CCCCATACCC CGGTGTGCCT GTGGAGGAAC TTTTCAAGCT GCTGAAGGAG 780  
GGTCACCGCA TGGACAAGCC CAGTAACTGC ACCAACGAGC TGTACATGAT GATGCGGGAC 840  
TGCTGGCATG CAGTGCCCTC ACAGAGACCC ACCTTCAAGC AGCTGGTGGA AGACCTGGAC 900  
CGCATCGTGG CCTTGACCTC CAACCAGGAG TAG 933

## (2) INFORMATION FOR SEQ ID NO:5:

## (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 1056 base pairs  
(B) TYPE: nucleic acid  
(C) STRANDEDNESS: double  
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: cDNA

## (xi) SEQUENCE DESCRIPTION: SEQ ID NO:5:

ATGCGGGGTT CTCATCATCA TCATCATCAT GGTATGGCTA GCATGACTGG TGGACAGCAA 60  
ATGGGTCTGGG ATCTGTACGA CGATGACGAT AAGGATCCGA GCTCGAGATC TGCAGCTGGT 120  
ACCATGGTAG CAGGGGTCTC TGAGTATGAG CTTCCCGAAG ACCCTCGCTG GGAGCTGCCT 180  
CGGGACAGAC TGGTCTTAGG CAAACCCCTG GGAGAGGGCG CCTTTGGGCA GGTGGTGTG 240  
GCAGAGGCTA TCGGGCTGGA CAAGGACAAA CCCAACCGTG TGACCAAAGT GGCTGTGAAG 300  
ATGTTGAAGT CGGACGCAAC AGAGAAAGAC TTGTCAGACC TGATCTCAGA AATGGAGATG 360  
ATGAAGATGA TCGGGAAGCA TAAGAATATC ATCAACCTGC TGGGGGCCTG CACGCAGGAT 420  
GGTCCCTTGT ATGTCATCGT GGAGTATGCC TCCAAGGGCA ACCTGCGGGA GTACCTGCAG 480  
GCCCCGAGGC CCCAGGGCT GGAATACTCC TACAACCCCA GCCACAACCC AGAGGAGCAG 540  
CTCTCCTCCA AGGACCTGGT GTCCTGCGCC TACCAGGTGG CCCGAGGCAT GGAGTATCTG 600  
GCCTCCAAGA AGTGCATACA CCGAGACCTG GCAGCCAGGA ATGTCCTGGT GACAGAGGAC 660

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AATGTGATGA AGATAGCAGA CTTTGGCCTC GCACGGGACA TTCACCACAT CGACTACTAT 720  
AAAAAGACAA CCAACGGCCG ACTGCCTGTG AAGTGGATGG CACCCGAGGC ATTATTTGAC 780  
CGGATCTACA CCCACCAGAG TGATGTGTGG TCTTTCGGGG TGCTCCTGTG GGAGATCTTC 840  
ACTCTGGGCG GCTCCCCATA CCCCAGGTGTG CCTGTGGAGG AACTTTTCAA GCTGCTGAAG 900  
GAGGGTCACC GCATGGACAA GCCCAGTAAC TGCACCAACG AGCTGTACAT GATGATGCGG 960  
GACTGCTGGC ATGCAGTGCC CTCACAGAGA CCCACCTTCA AGCAGCTGGT GGAAGACCTG 1020  
GACCGCATCG TGGCCTTGAC CTCCAACCAG GAGTAG 1056

TABLE 1

Atom No.	Atom Type	A.A	A.A No.	X	Y	Z	OCC	B
ATOM 1	N	GLU	1464	-13.639	16.975	8.571	1.00	54.29
ATOM 3	CA	GLU	1464	-12.479	17.105	7.695	1.00	52.62
ATOM 4	CB	GLU	1464	-11.400	17.974	8.349	1.00	54.64
ATOM 5	C	GLU	1464	-11.914	15.738	7.319	1.00	49.74
ATOM 6	O	GLU	1464	-11.845	15.407	6.136	1.00	52.04
ATOM 7	N	LEU	1465	-11.562	14.925	8.310	1.00	44.95
ATOM 9	CA	LEU	1465	-11.018	13.599	8.037	1.00	41.04
ATOM 10	CB	LEU	1465	-10.236	13.066	9.235	1.00	40.18
ATOM 11	CG	LEU	1465	-8.719	13.196	9.130	1.00	43.70
ATOM 12	CD1	LEU	1465	-8.346	14.654	8.891	1.00	46.74
ATOM 13	CD2	LEU	1465	-8.061	12.671	10.395	1.00	40.72
ATOM 14	C	LEU	1465	-12.092	12.594	7.656	1.00	39.18
ATOM 15	O	LEU	1465	-13.187	12.590	8.219	1.00	38.05
ATOM 16	N	PRO	1466	-11.802	11.748	6.657	1.00	37.20
ATOM 17	CD	PRO	1466	-10.597	11.793	5.810	1.00	36.41
ATOM 18	CA	PRO	1466	-12.741	10.727	6.189	1.00	36.13
ATOM 19	CB	PRO	1466	-12.110	10.262	4.878	1.00	37.50
ATOM 20	CG	PRO	1466	-10.629	10.459	5.135	1.00	36.20
ATOM 21	C	PRO	1466	-12.846	9.595	7.201	1.00	35.61
ATOM 22	O	PRO	1466	-11.847	9.174	7.788	1.00	35.18
ATOM 23	N	GLU	1467	-14.060	9.121	7.429	1.00	35.38
ATOM 25	CA	GLU	1467	-14.268	8.053	8.377	1.00	35.43
ATOM 26	CB	GLU	1467	-15.744	7.965	8.746	1.00	41.10
ATOM 27	CG	GLU	1467	-16.375	9.280	9.098	1.00	48.25
ATOM 28	CD	GLU	1467	-17.819	9.145	9.596	1.00	50.24
ATOM 29	OE1	GLU	1467	-18.446	8.071	9.378	1.00	52.82
ATOM 30	OE2	GLU	1467	-18.314	10.109	10.230	1.00	51.26
ATOM 31	C	GLU	1467	-13.838	6.714	7.801	1.00	32.65
ATOM 32	O	GLU	1467	-13.899	6.511	6.591	1.00	35.06
ATOM 33	N	ASP	1468	-13.299	5.854	8.659	1.00	30.46
ATOM 35	CA	ASP	1468	-12.883	4.516	8.262	1.00	28.85
ATOM 36	CB	ASP	1468	-11.384	4.424	7.975	1.00	29.34
ATOM 37	CG	ASP	1468	-10.985	3.072	7.408	1.00	27.57
ATOM 38	OD1	ASP	1468	-11.833	2.159	7.359	1.00	27.78
ATOM 39	OD2	ASP	1468	-9.817	2.916	7.003	1.00	30.64
ATOM 40	C	ASP	1468	-13.252	3.564	9.384	1.00	29.29
ATOM 41	O	ASP	1468	-12.481	3.364	10.336	1.00	27.76
ATOM 42	N	PRO	1469	-14.435	2.939	9.268	1.00	28.99
ATOM 43	CD	PRO	1469	-15.354	3.091	8.120	1.00	28.09
ATOM 44	CA	PRO	1469	-14.971	1.987	10.244	1.00	30.01
ATOM 45	CB	PRO	1469	-16.244	1.473	9.553	1.00	33.33
ATOM 46	CG	PRO	1469	-16.665	2.630	8.690	1.00	30.53
ATOM 47	C	PRO	1469	-14.012	0.848	10.563	1.00	28.96
ATOM 48	O	PRO	1469	-14.085	0.251	11.636	1.00	28.52
ATOM 49	N	ARG	1470	-13.106	0.556	9.631	1.00	27.59
ATOM 51	CA	ARG	1470	-12.139	-0.520	9.810	1.00	27.37
ATOM 52	CB	ARG	1470	-11.301	-0.707	8.533	1.00	28.84

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ATOM	53	CG	ARG	1470	-12.049	-1.279	7.317	1.00	30.57
ATOM	54	CD	ARG	1470	-11.137	-1.352	6.068	1.00	26.71
ATOM	55	NE	ARG	1470	-10.489	-0.068	5.793	1.00	31.26
ATOM	57	CZ	ARG	1470	-9.603	0.151	4.823	1.00	32.60
ATOM	58	NH1	ARG	1470	-9.241	-0.828	3.999	1.00	33.19
ATOM	61	NH2	ARG	1470	-9.067	1.359	4.686	1.00	28.65
ATOM	64	C	ARG	1470	-11.180	-0.285	10.981	1.00	29.21
ATOM	65	O	ARG	1470	-10.757	-1.230	11.641	1.00	28.47
ATOM	66	N	TRP	1471	-10.909	0.977	11.280	1.00	27.80
ATOM	68	CA	TRP	1471	-9.940	1.314	12.306	1.00	28.62
ATOM	69	CB	TRP	1471	-8.729	1.944	11.609	1.00	24.97
ATOM	70	CG	TRP	1471	-8.044	0.976	10.728	1.00	24.86
ATOM	71	CD2	TRP	1471	-7.156	-0.060	11.144	1.00	28.00
ATOM	72	CE2	TRP	1471	-6.782	-0.776	9.989	1.00	29.23
ATOM	73	CE3	TRP	1471	-6.642	-0.460	12.389	1.00	26.59
ATOM	74	CD1	TRP	1471	-8.166	0.860	9.374	1.00	27.23
ATOM	75	NE1	TRP	1471	-7.413	-0.192	8.922	1.00	30.10
ATOM	77	CZ2	TRP	1471	-5.912	-1.866	10.036	1.00	28.70
ATOM	78	CZ3	TRP	1471	-5.778	-1.545	12.435	1.00	27.18
ATOM	79	CH2	TRP	1471	-5.424	-2.237	11.266	1.00	27.23
ATOM	80	C	TRP	1471	-10.371	2.223	13.440	1.00	28.42
ATOM	81	O	TRP	1471	-9.664	2.321	14.442	1.00	26.48
ATOM	82	N	GLU	1472	-11.521	2.874	13.293	1.00	28.62
ATOM	84	CA	GLU	1472	-11.981	3.823	14.297	1.00	27.16
ATOM	85	CB	GLU	1472	-13.245	4.534	13.799	1.00	28.89
ATOM	86	CG	GLU	1472	-13.552	5.869	14.520	1.00	29.09
ATOM	87	CD	GLU	1472	-12.692	7.042	14.054	1.00	26.43
ATOM	88	OE1	GLU	1472	-12.134	7.009	12.938	1.00	28.59
ATOM	89	OE2	GLU	1472	-12.596	8.024	14.801	1.00	27.28
ATOM	90	C	GLU	1472	-12.217	3.269	15.701	1.00	25.10
ATOM	91	O	GLU	1472	-12.763	2.196	15.861	1.00	26.48
ATOM	92	N	LEU	1473	-11.750	3.991	16.711	1.00	24.65
ATOM	94	CA	LEU	1473	-11.962	3.608	18.104	1.00	26.27
ATOM	95	CB	LEU	1473	-10.645	3.266	18.817	1.00	28.24
ATOM	96	CG	LEU	1473	-10.750	3.025	20.337	1.00	27.23
ATOM	97	CD1	LEU	1473	-11.323	1.636	20.642	1.00	25.23
ATOM	98	CD2	LEU	1473	-9.390	3.183	21.000	1.00	26.33
ATOM	99	C	LEU	1473	-12.546	4.856	18.740	1.00	26.52
ATOM	100	O	LEU	1473	-12.122	5.973	18.411	1.00	25.16
ATOM	101	N	PRO	1474	-13.610	4.703	19.554	1.00	28.52
ATOM	102	CD	PRO	1474	-14.435	3.500	19.770	1.00	29.65
ATOM	103	CA	PRO	1474	-14.215	5.870	20.207	1.00	29.18
ATOM	104	CB	PRO	1474	-15.368	5.251	21.003	1.00	28.58
ATOM	105	CG	PRO	1474	-15.768	4.097	20.154	1.00	28.17
ATOM	106	C	PRO	1474	-13.173	6.528	21.124	1.00	29.75
ATOM	107	O	PRO	1474	-12.427	5.841	21.828	1.00	31.78
ATOM	108	N	ARG	1475	-13.107	7.849	21.097	1.00	30.76
ATOM	110	CA	ARG	1475	-12.149	8.588	21.900	1.00	32.26
ATOM	111	CB	ARG	1475	-12.362	10.083	21.743	1.00	31.58
ATOM	112	CG	ARG	1475	-12.178	10.536	20.342	1.00	37.54
ATOM	113	CD	ARG	1475	-12.048	12.027	20.206	1.00	36.96
ATOM	114	NE	ARG	1475	-11.733	12.317	18.813	1.00	40.07
ATOM	116	CZ	ARG	1475	-10.503	12.501	18.352	1.00	37.59
ATOM	117	NH1	ARG	1475	-9.470	12.447	19.186	1.00	34.89

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ATOM	120	NH2	ARG	1475	-10.308	12.669	17.049	1.00	34.54
ATOM	123	C	ARG	1475	-12.173	8.261	23.371	1.00	35.58
ATOM	124	O	ARG	1475	-11.135	8.318	24.036	1.00	37.03
ATOM	125	N	ASP	1476	-13.356	7.958	23.889	1.00	36.68
ATOM	127	CA	ASP	1476	-13.498	7.647	25.307	1.00	37.07
ATOM	128	CB	ASP	1476	-14.967	7.759	25.740	1.00	37.87
ATOM	129	CG	ASP	1476	-15.851	6.704	25.115	1.00	38.93
ATOM	130	OD1	ASP	1476	-15.412	6.015	24.179	1.00	43.75
ATOM	131	OD2	ASP	1476	-17.003	6.558	25.563	1.00	45.77
ATOM	132	C	ASP	1476	-12.922	6.292	25.701	1.00	35.86
ATOM	133	O	ASP	1476	-12.923	5.928	26.878	1.00	37.98
ATOM	134	N	ARG	1477	-12.478	5.527	24.711	1.00	33.37
ATOM	136	CA	ARG	1477	-11.889	4.221	24.961	1.00	31.84
ATOM	137	CB	ARG	1477	-12.214	3.262	23.809	1.00	31.84
ATOM	138	CG	ARG	1477	-13.693	2.965	23.580	1.00	29.70
ATOM	139	CD	ARG	1477	-14.366	2.365	24.809	1.00	33.88
ATOM	140	NE	ARG	1477	-14.596	3.372	25.838	1.00	33.86
ATOM	142	CZ	ARG	1477	-14.845	3.102	27.113	1.00	34.14
ATOM	143	NH1	ARG	1477	-14.906	1.846	27.542	1.00	30.58
ATOM	146	NH2	ARG	1477	-15.024	4.102	27.961	1.00	33.14
ATOM	149	C	ARG	1477	-10.373	4.338	25.105	1.00	31.30
ATOM	150	O	ARG	1477	-9.679	3.362	25.365	1.00	32.32
ATOM	151	N	LEU	1478	-9.856	5.544	24.978	1.00	32.85
ATOM	153	CA	LEU	1478	-8.426	5.739	25.054	1.00	35.64
ATOM	154	CB	LEU	1478	-7.964	6.360	23.737	1.00	34.96
ATOM	155	CG	LEU	1478	-6.498	6.291	23.331	1.00	36.36
ATOM	156	CD1	LEU	1478	-6.059	4.833	23.192	1.00	30.71
ATOM	157	CD2	LEU	1478	-6.335	7.048	22.020	1.00	33.97
ATOM	158	C	LEU	1478	-8.054	6.625	26.243	1.00	37.60
ATOM	159	O	LEU	1478	-8.366	7.815	26.263	1.00	41.20
ATOM	160	N	VAL	1479	-7.442	6.023	27.257	1.00	36.52
ATOM	162	CA	VAL	1479	-7.008	6.745	28.449	1.00	35.59
ATOM	163	CB	VAL	1479	-7.041	5.829	29.688	1.00	35.92
ATOM	164	CG1	VAL	1479	-6.712	6.627	30.926	1.00	39.40
ATOM	165	CG2	VAL	1479	-8.404	5.163	29.825	1.00	34.46
ATOM	166	C	VAL	1479	-5.577	7.224	28.197	1.00	35.36
ATOM	167	O	VAL	1479	-4.622	6.443	28.269	1.00	32.50
ATOM	168	N	LEU	1480	-5.439	8.506	27.878	1.00	37.77
ATOM	170	CA	LEU	1480	-4.132	9.086	27.572	1.00	42.77
ATOM	171	CB	LEU	1480	-4.298	10.421	26.842	1.00	41.84
ATOM	172	CG	LEU	1480	-4.991	10.369	25.471	1.00	42.45
ATOM	173	CD1	LEU	1480	-5.135	11.774	24.924	1.00	42.58
ATOM	174	CD2	LEU	1480	-4.200	9.508	24.502	1.00	43.09
ATOM	175	C	LEU	1480	-3.211	9.233	28.778	1.00	45.25
ATOM	176	O	LEU	1480	-3.621	9.739	29.822	1.00	45.47
ATOM	177	N	GLY	1481	-1.958	8.816	28.612	1.00	46.82
ATOM	179	CA	GLY	1481	-1.016	8.889	29.708	1.00	50.47
ATOM	180	C	GLY	1481	0.296	9.617	29.472	1.00	52.24
ATOM	181	O	GLY	1481	0.360	10.638	28.781	1.00	53.41
ATOM	182	N	LYS	1482	1.349	9.070	30.068	1.00	53.64
ATOM	184	CA	LYS	1482	2.697	9.627	30.000	1.00	56.19
ATOM	185	CB	LYS	1482	3.636	8.776	30.859	1.00	57.19
ATOM	186	CG	LYS	1482	5.115	9.023	30.628	1.00	61.02
ATOM	187	CD	LYS	1482	5.938	7.831	31.089	1.00	63.12

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ATOM	188	CE	LYS	1482	5.494	6.547	30.395	1.00	61.98
ATOM	189	NZ	LYS	1482	6.252	5.368	30.899	1.00	63.38
ATOM	193	C	LYS	1482	3.297	9.795	28.604	1.00	56.56
ATOM	194	O	LYS	1482	3.291	8.868	27.791	1.00	55.03
ATOM	195	N	PRO	1483	3.852	10.983	28.323	1.00	58.31
ATOM	196	CD	PRO	1483	3.859	12.191	29.167	1.00	56.98
ATOM	197	CA	PRO	1483	4.465	11.254	27.020	1.00	59.52
ATOM	198	CB	PRO	1483	4.910	12.711	27.155	1.00	58.75
ATOM	199	CG	PRO	1483	3.927	13.278	28.141	1.00	58.79
ATOM	200	C	PRO	1483	5.673	10.335	26.834	1.00	61.17
ATOM	201	O	PRO	1483	6.509	10.216	27.731	1.00	61.31
ATOM	202	N	LEU	1484	5.728	9.643	25.702	1.00	64.31
ATOM	204	CA	LEU	1484	6.838	8.738	25.408	1.00	67.77
ATOM	205	CB	LEU	1484	6.349	7.512	24.640	1.00	67.66
ATOM	206	CG	LEU	1484	5.415	6.558	25.386	1.00	69.00
ATOM	207	CD1	LEU	1484	4.943	5.457	24.445	1.00	66.76
ATOM	208	CD2	LEU	1484	6.126	5.972	26.604	1.00	67.77
ATOM	209	C	LEU	1484	7.934	9.431	24.608	1.00	70.82
ATOM	210	O	LEU	1484	9.117	9.115	24.759	1.00	71.82
ATOM	211	N	GLY	1485	7.534	10.357	23.742	1.00	73.28
ATOM	213	CA	GLY	1485	8.492	11.077	22.922	1.00	74.53
ATOM	214	C	GLY	1485	7.819	11.754	21.747	1.00	75.19
ATOM	215	O	GLY	1485	6.635	12.090	21.822	1.00	75.61
ATOM	216	N	GLN	1491	4.406	14.274	18.638	1.00	50.72
ATOM	218	CA	GLN	1491	4.042	13.876	19.994	1.00	47.33
ATOM	219	CB	GLN	1491	3.033	14.869	20.587	1.00	46.67
ATOM	220	C	GLN	1491	3.486	12.449	20.073	1.00	46.66
ATOM	221	O	GLN	1491	2.581	12.074	19.323	1.00	45.20
ATOM	222	N	VAL	1492	4.072	11.650	20.960	1.00	45.41
ATOM	224	CA	VAL	1492	3.646	10.274	21.184	1.00	43.83
ATOM	225	CB	VAL	1492	4.680	9.244	20.709	1.00	41.60
ATOM	226	CG1	VAL	1492	4.138	7.849	20.937	1.00	41.35
ATOM	227	CG2	VAL	1492	5.007	9.445	19.237	1.00	42.72
ATOM	228	C	VAL	1492	3.458	10.084	22.683	1.00	44.45
ATOM	229	O	VAL	1492	4.335	10.437	23.482	1.00	43.86
ATOM	230	N	VAL	1493	2.309	9.548	23.070	1.00	42.67
ATOM	232	CA	VAL	1493	2.029	9.321	24.477	1.00	41.05
ATOM	233	CB	VAL	1493	0.884	10.242	25.013	1.00	40.64
ATOM	234	CG1	VAL	1493	1.177	11.693	24.722	1.00	42.40
ATOM	235	CG2	VAL	1493	-0.459	9.844	24.427	1.00	43.36
ATOM	236	C	VAL	1493	1.626	7.880	24.704	1.00	40.09
ATOM	237	O	VAL	1493	1.129	7.212	23.796	1.00	39.99
ATOM	238	N	LEU	1494	1.927	7.374	25.890	1.00	37.10
ATOM	240	CA	LEU	1494	1.535	6.036	26.250	1.00	35.08
ATOM	241	CB	LEU	1494	2.359	5.542	27.440	1.00	35.57
ATOM	242	CG	LEU	1494	2.036	4.161	28.007	1.00	36.87
ATOM	243	CD1	LEU	1494	2.123	3.085	26.931	1.00	36.90
ATOM	244	CD2	LEU	1494	2.998	3.860	29.143	1.00	41.99
ATOM	245	C	LEU	1494	0.077	6.236	26.648	1.00	33.31
ATOM	246	O	LEU	1494	-0.311	7.318	27.097	1.00	32.93
ATOM	247	N	ALA	1495	-0.740	5.219	26.435	1.00	33.35
ATOM	249	CA	ALA	1495	-2.147	5.292	26.773	1.00	30.67
ATOM	250	CB	ALA	1495	-2.923	5.937	25.637	1.00	30.35
ATOM	251	C	ALA	1495	-2.661	3.893	27.025	1.00	29.97

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ATOM	252	O	ALA	1495	-1.944	2.909	26.840	1.00	28.15
ATOM	253	N	GLU	1496	-3.898	3.813	27.488	1.00	30.37
ATOM	255	CA	GLU	1496	-4.537	2.536	27.745	1.00	31.47
ATOM	256	CB	GLU	1496	-4.862	2.392	29.223	1.00	32.48
ATOM	257	CG	GLU	1496	-3.627	2.239	30.093	1.00	37.81
ATOM	258	CD	GLU	1496	-3.938	2.426	31.565	1.00	41.09
ATOM	259	OE1	GLU	1496	-4.328	3.548	31.944	1.00	41.53
ATOM	260	OE2	GLU	1496	-3.797	1.453	32.341	1.00	44.12
ATOM	261	C	GLU	1496	-5.806	2.524	26.916	1.00	32.72
ATOM	262	O	GLU	1496	-6.586	3.478	26.954	1.00	33.91
ATOM	263	N	ALA	1497	-5.953	1.494	26.094	1.00	31.06
ATOM	265	CA	ALA	1497	-7.117	1.353	25.239	1.00	32.33
ATOM	266	CB	ALA	1497	-6.691	0.879	23.859	1.00	29.56
ATOM	267	C	ALA	1497	-8.056	0.343	25.885	1.00	32.26
ATOM	268	O	ALA	1497	-7.648	-0.773	26.197	1.00	33.55
ATOM	269	N	ILE	1498	-9.286	0.759	26.160	1.00	32.99
ATOM	271	CA	ILE	1498	-10.276	-0.126	26.766	1.00	34.00
ATOM	272	CB	ILE	1498	-11.329	0.668	27.592	1.00	34.69
ATOM	273	CG2	ILE	1498	-12.341	-0.288	28.240	1.00	34.24
ATOM	274	CG1	ILE	1498	-10.647	1.496	28.686	1.00	33.56
ATOM	275	CD1	ILE	1498	-11.543	2.572	29.258	1.00	31.25
ATOM	276	C	ILE	1498	-10.994	-0.830	25.624	1.00	35.71
ATOM	277	O	ILE	1498	-11.618	-0.181	24.786	1.00	34.88
ATOM	278	N	GLY	1499	-10.890	-2.147	25.573	1.00	40.43
ATOM	280	CA	GLY	1499	-11.553	-2.884	24.516	1.00	47.63
ATOM	281	C	GLY	1499	-10.670	-3.233	23.330	1.00	53.08
ATOM	282	O	GLY	1499	-9.934	-4.226	23.380	1.00	54.97
ATOM	283	N	LEU	1500	-10.713	-2.394	22.294	1.00	54.18
ATOM	285	CA	LEU	1500	-9.957	-2.603	21.055	1.00	55.26
ATOM	286	CB	LEU	1500	-8.444	-2.726	21.305	1.00	55.39
ATOM	287	CG	LEU	1500	-7.562	-1.472	21.241	1.00	54.27
ATOM	288	CD1	LEU	1500	-6.110	-1.891	21.367	1.00	52.89
ATOM	289	CD2	LEU	1500	-7.768	-0.711	19.935	1.00	50.91
ATOM	290	C	LEU	1500	-10.453	-3.830	20.288	1.00	55.39
ATOM	291	O	LEU	1500	-10.376	-4.963	20.774	1.00	56.23
ATOM	292	N	PRO	1505	-13.315	-5.836	25.394	1.00	53.03
ATOM	293	CD	PRO	1505	-13.945	-7.148	25.167	1.00	55.12
ATOM	294	CA	PRO	1505	-14.306	-4.848	25.846	1.00	50.62
ATOM	295	CB	PRO	1505	-15.635	-5.607	25.715	1.00	50.09
ATOM	296	CG	PRO	1505	-15.241	-7.031	25.950	1.00	52.18
ATOM	297	C	PRO	1505	-14.039	-4.348	27.273	1.00	46.35
ATOM	298	O	PRO	1505	-14.065	-3.143	27.524	1.00	45.82
ATOM	299	N	ASN	1506	-13.711	-5.261	28.181	1.00	42.76
ATOM	301	CA	ASN	1506	-13.433	-4.892	29.566	1.00	45.29
ATOM	302	CB	ASN	1506	-14.283	-5.728	30.529	1.00	45.92
ATOM	303	CG	ASN	1506	-15.752	-5.395	30.441	1.00	46.17
ATOM	304	OD1	ASN	1506	-16.132	-4.232	30.390	1.00	48.57
ATOM	305	ND2	ASN	1506	-16.589	-6.418	30.406	1.00	48.63
ATOM	308	C	ASN	1506	-11.954	-5.008	29.939	1.00	45.33
ATOM	309	O	ASN	1506	-11.597	-5.084	31.121	1.00	44.53
ATOM	310	N	ARG	1507	-11.100	-5.010	28.924	1.00	45.63
ATOM	312	CA	ARG	1507	-9.660	-5.122	29.117	1.00	45.57
ATOM	313	CB	ARG	1507	-9.131	-6.354	28.375	1.00	53.33
ATOM	314	CG	ARG	1507	-9.407	-7.685	29.043	1.00	61.39

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ATOM	315	CD	ARG	1507	-8.336	-8.028	30.063	1.00	67.74
ATOM	316	NE	ARG	1507	-8.525	-9.376	30.585	1.00	74.64
ATOM	318	CZ	ARG	1507	-7.970	-9.842	31.701	1.00	80.01
ATOM	319	NH1	ARG	1507	-7.166	-9.075	32.433	1.00	80.04
ATOM	322	NH2	ARG	1507	-8.268	-11.068	32.115	1.00	83.41
ATOM	325	C	ARG	1507	-8.964	-3.897	28.555	1.00	40.94
ATOM	326	O	ARG	1507	-9.370	-3.375	27.517	1.00	37.60
ATOM	327	N	VAL	1508	-7.956	-3.409	29.267	1.00	39.33
ATOM	329	CA	VAL	1508	-7.190	-2.269	28.789	1.00	37.26
ATOM	330	CB	VAL	1508	-6.854	-1.224	29.905	1.00	36.25
ATOM	331	CG1	VAL	1508	-8.124	-0.739	30.571	1.00	39.63
ATOM	332	CG2	VAL	1508	-5.903	-1.796	30.928	1.00	36.92
ATOM	333	C	VAL	1508	-5.898	-2.818	28.188	1.00	34.38
ATOM	334	O	VAL	1508	-5.387	-3.851	28.630	1.00	32.85
ATOM	335	N	THR	1509	-5.406	-2.140	27.159	1.00	30.47
ATOM	337	CA	THR	1509	-4.174	-2.523	26.491	1.00	31.65
ATOM	338	CB	THR	1509	-4.455	-2.959	25.027	1.00	34.13
ATOM	339	OG1	THR	1509	-5.426	-4.013	25.018	1.00	40.74
ATOM	341	CG2	THR	1509	-3.184	-3.458	24.345	1.00	31.06
ATOM	342	C	THR	1509	-3.270	-1.299	26.461	1.00	28.38
ATOM	343	O	THR	1509	-3.716	-0.219	26.104	1.00	27.78
ATOM	344	N	LYS	1510	-2.023	-1.442	26.896	1.00	29.48
ATOM	346	CA	LYS	1510	-1.101	-0.312	26.835	1.00	30.54
ATOM	347	CB	LYS	1510	0.172	-0.558	27.635	1.00	27.88
ATOM	348	CG	LYS	1510	-0.037	-0.600	29.118	1.00	33.91
ATOM	349	CD	LYS	1510	1.284	-0.759	29.840	1.00	40.30
ATOM	350	CE	LYS	1510	1.145	-1.674	31.062	1.00	46.24
ATOM	351	NZ	LYS	1510	0.338	-1.096	32.187	1.00	49.09
ATOM	355	C	LYS	1510	-0.757	-0.166	25.365	1.00	28.64
ATOM	356	O	LYS	1510	-0.402	-1.142	24.704	1.00	28.76
ATOM	357	N	VAL	1511	-0.902	1.048	24.856	1.00	29.34
ATOM	359	CA	VAL	1511	-0.627	1.347	23.463	1.00	29.79
ATOM	360	CB	VAL	1511	-1.951	1.457	22.658	1.00	27.14
ATOM	361	CG1	VAL	1511	-2.681	0.111	22.657	1.00	24.56
ATOM	362	CG2	VAL	1511	-2.837	2.561	23.243	1.00	22.15
ATOM	363	C	VAL	1511	0.123	2.672	23.361	1.00	29.83
ATOM	364	O	VAL	1511	0.213	3.413	24.338	1.00	33.14
ATOM	365	N	ALA	1512	0.705	2.939	22.196	1.00	27.86
ATOM	367	CA	ALA	1512	1.405	4.192	21.962	1.00	25.55
ATOM	368	CB	ALA	1512	2.743	3.935	21.297	1.00	24.69
ATOM	369	C	ALA	1512	0.500	5.009	21.057	1.00	25.25
ATOM	370	O	ALA	1512	-0.061	4.483	20.107	1.00	27.18
ATOM	371	N	VAL	1513	0.340	6.289	21.360	1.00	29.63
ATOM	373	CA	VAL	1513	-0.520	7.165	20.573	1.00	32.66
ATOM	374	CB	VAL	1513	-1.704	7.713	21.422	1.00	32.47
ATOM	375	CG1	VAL	1513	-2.609	8.585	20.574	1.00	32.29
ATOM	376	CG2	VAL	1513	-2.508	6.559	22.031	1.00	32.15
ATOM	377	C	VAL	1513	0.238	8.334	19.938	1.00	34.67
ATOM	378	O	VAL	1513	0.792	9.185	20.635	1.00	34.65
ATOM	379	N	LYS	1514	0.207	8.367	18.605	1.00	36.88
ATOM	381	CA	LYS	1514	0.859	9.390	17.789	1.00	36.43
ATOM	382	CB	LYS	1514	1.349	8.764	16.489	1.00	36.37
ATOM	383	CG	LYS	1514	2.250	7.563	16.697	1.00	39.49
ATOM	384	CD	LYS	1514	2.559	6.854	15.390	1.00	45.29

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ATOM	385	CE	LYS	1514	3.080	7.815	14.331	1.00	50.70
ATOM	386	NZ	LYS	1514	4.212	8.685	14.798	1.00	51.41
ATOM	390	C	LYS	1514	-0.121	10.496	17.459	1.00	36.75
ATOM	391	O	LYS	1514	-1.228	10.234	16.978	1.00	35.42
ATOM	392	N	MET	1515	0.294	11.731	17.700	1.00	38.12
ATOM	394	CA	MET	1515	-0.545	12.882	17.432	1.00	41.90
ATOM	395	CB	MET	1515	-1.371	13.238	18.668	1.00	43.08
ATOM	396	CG	MET	1515	-0.536	13.601	19.880	1.00	45.01
ATOM	397	SD	MET	1515	-1.561	13.784	21.324	1.00	46.03
ATOM	398	CE	MET	1515	-1.675	12.072	21.885	1.00	44.02
ATOM	399	C	MET	1515	0.314	14.065	17.021	1.00	44.65
ATOM	400	O	MET	1515	1.543	14.013	17.094	1.00	45.64
ATOM	401	N	LEU	1516	-0.347	15.123	16.568	1.00	47.08
ATOM	403	CA	LEU	1516	0.329	16.337	16.134	1.00	48.08
ATOM	404	CB	LEU	1516	-0.500	17.033	15.054	1.00	45.50
ATOM	405	CG	LEU	1516	-0.764	16.265	13.764	1.00	43.22
ATOM	406	CD1	LEU	1516	-1.783	17.014	12.946	1.00	40.32
ATOM	407	CD2	LEU	1516	0.540	16.072	12.991	1.00	43.78
ATOM	408	C	LEU	1516	0.516	17.302	17.297	1.00	51.27
ATOM	409	O	LEU	1516	-0.214	17.249	18.291	1.00	50.37
ATOM	410	N	LYS	1517	1.491	18.191	17.157	1.00	55.47
ATOM	412	CA	LYS	1517	1.757	19.207	18.168	1.00	59.10
ATOM	413	CB	LYS	1517	3.203	19.702	18.068	1.00	61.61
ATOM	414	CG	LYS	1517	4.251	18.669	18.462	1.00	64.82
ATOM	415	CD	LYS	1517	5.635	19.109	18.018	1.00	67.42
ATOM	416	CE	LYS	1517	6.696	18.102	18.432	1.00	71.76
ATOM	417	NZ	LYS	1517	8.021	18.411	17.812	1.00	73.57
ATOM	421	C	LYS	1517	0.794	20.365	17.920	1.00	59.91
ATOM	422	O	LYS	1517	0.187	20.456	16.852	1.00	59.88
ATOM	423	N	SER	1518	0.686	21.267	18.886	1.00	61.85
ATOM	425	CA	SER	1518	-0.216	22.409	18.760	1.00	63.70
ATOM	426	CB	SER	1518	-0.158	23.274	20.024	1.00	64.21
ATOM	427	C	SER	1518	0.079	23.263	17.529	1.00	64.37
ATOM	428	O	SER	1518	-0.841	23.757	16.875	1.00	66.16
ATOM	429	N	ASP	1519	1.359	23.410	17.202	1.00	64.15
ATOM	431	CA	ASP	1519	1.767	24.217	16.054	1.00	64.55
ATOM	432	CB	ASP	1519	3.109	24.897	16.343	1.00	65.84
ATOM	433	C	ASP	1519	1.858	23.441	14.742	1.00	63.95
ATOM	434	O	ASP	1519	2.432	23.931	13.769	1.00	64.95
ATOM	435	N	ALA	1520	1.303	22.232	14.719	1.00	62.57
ATOM	437	CA	ALA	1520	1.329	21.398	13.521	1.00	60.34
ATOM	438	CB	ALA	1520	0.704	20.039	13.810	1.00	60.53
ATOM	439	C	ALA	1520	0.616	22.062	12.353	1.00	58.21
ATOM	440	O	ALA	1520	-0.464	22.631	12.506	1.00	58.32
ATOM	441	N	THR	1521	1.241	22.001	11.186	1.00	55.96
ATOM	443	CA	THR	1521	0.673	22.582	9.981	1.00	54.98
ATOM	444	CB	THR	1521	1.783	23.013	9.031	1.00	53.84
ATOM	445	OG1	THR	1521	2.554	21.862	8.659	1.00	55.84
ATOM	447	CG2	THR	1521	2.693	24.026	9.703	1.00	55.01
ATOM	448	C	THR	1521	-0.184	21.545	9.261	1.00	54.25
ATOM	449	O	THR	1521	-0.190	20.371	9.629	1.00	54.74
ATOM	450	N	GLU	1522	-0.877	21.974	8.212	1.00	53.32
ATOM	452	CA	GLU	1522	-1.702	21.066	7.423	1.00	52.64
ATOM	453	CB	GLU	1522	-2.472	21.829	6.339	1.00	53.55

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ATOM	454	C	GLU	1522	-0.793	20.012	6.780	1.00	51.95
ATOM	455	O	GLU	1522	-1.226	18.895	6.504	1.00	53.28
ATOM	456	N	LYS	1523	0.464	20.377	6.544	1.00	48.66
ATOM	458	CA	LYS	1523	1.429	19.460	5.963	1.00	46.30
ATOM	459	CB	LYS	1523	2.730	20.201	5.620	1.00	48.30
ATOM	460	CG	LYS	1523	3.889	19.308	5.164	1.00	49.58
ATOM	461	CD	LYS	1523	3.487	18.388	4.016	1.00	50.87
ATOM	462	CE	LYS	1523	4.688	17.635	3.466	1.00	54.08
ATOM	463	NZ	LYS	1523	4.271	16.629	2.440	1.00	57.87
ATOM	467	C	LYS	1523	1.699	18.391	7.006	1.00	43.89
ATOM	468	O	LYS	1523	1.747	17.202	6.697	1.00	43.92
ATOM	469	N	ASP	1524	1.857	18.828	8.249	1.00	42.71
ATOM	471	CA	ASP	1524	2.114	17.915	9.351	1.00	42.11
ATOM	472	CB	ASP	1524	2.313	18.701	10.653	1.00	44.94
ATOM	473	CG	ASP	1524	3.623	19.490	10.673	1.00	48.90
ATOM	474	OD1	ASP	1524	3.692	20.512	11.392	1.00	51.88
ATOM	475	OD2	ASP	1524	4.590	19.084	9.990	1.00	50.06
ATOM	476	C	ASP	1524	0.956	16.931	9.481	1.00	39.85
ATOM	477	O	ASP	1524	1.164	15.738	9.748	1.00	39.01
ATOM	478	N	LEU	1525	-0.261	17.438	9.296	1.00	38.32
ATOM	480	CA	LEU	1525	-1.461	16.610	9.355	1.00	36.16
ATOM	481	CB	LEU	1525	-2.720	17.470	9.200	1.00	35.13
ATOM	482	CG	LEU	1525	-4.081	16.760	9.186	1.00	34.70
ATOM	483	CD1	LEU	1525	-4.184	15.668	10.252	1.00	36.15
ATOM	484	CD2	LEU	1525	-5.162	17.789	9.395	1.00	32.96
ATOM	485	C	LEU	1525	-1.406	15.560	8.254	1.00	34.31
ATOM	486	O	LEU	1525	-1.575	14.377	8.518	1.00	33.34
ATOM	487	N	SER	1526	-1.136	16.005	7.030	1.00	36.40
ATOM	489	CA	SER	1526	-1.039	15.128	5.865	1.00	37.16
ATOM	490	CB	SER	1526	-0.669	15.931	4.618	1.00	38.84
ATOM	491	OG	SER	1526	-1.736	16.779	4.245	1.00	49.61
ATOM	493	C	SER	1526	-0.021	14.016	6.044	1.00	35.90
ATOM	494	O	SER	1526	-0.273	12.873	5.670	1.00	36.68
ATOM	495	N	ASP	1527	1.142	14.349	6.591	1.00	35.89
ATOM	497	CA	ASP	1527	2.177	13.342	6.796	1.00	35.25
ATOM	498	CB	ASP	1527	3.497	13.998	7.201	1.00	35.58
ATOM	499	CG	ASP	1527	4.100	14.850	6.081	1.00	37.19
ATOM	500	OD1	ASP	1527	3.750	14.653	4.895	1.00	37.38
ATOM	501	OD2	ASP	1527	4.932	15.726	6.395	1.00	42.93
ATOM	502	C	ASP	1527	1.749	12.274	7.799	1.00	31.77
ATOM	503	O	ASP	1527	2.000	11.090	7.594	1.00	30.58
ATOM	504	N	LEU	1528	1.055	12.684	8.853	1.00	31.80
ATOM	506	CA	LEU	1528	0.581	11.730	9.857	1.00	33.53
ATOM	507	CB	LEU	1528	-0.002	12.471	11.076	1.00	32.20
ATOM	508	CG	LEU	1528	-0.440	11.623	12.275	1.00	32.63
ATOM	509	CD1	LEU	1528	0.705	10.708	12.709	1.00	33.09
ATOM	510	CD2	LEU	1528	-0.891	12.512	13.426	1.00	31.52
ATOM	511	C	LEU	1528	-0.468	10.792	9.235	1.00	32.89
ATOM	512	O	LEU	1528	-0.494	9.589	9.521	1.00	32.39
ATOM	513	N	ILE	1529	-1.336	11.357	8.393	1.00	33.72
ATOM	515	CA	ILE	1529	-2.376	10.591	7.711	1.00	30.48
ATOM	516	CB	ILE	1529	-3.336	11.505	6.895	1.00	28.85
ATOM	517	CG2	ILE	1529	-4.229	10.662	5.997	1.00	28.54
ATOM	518	CG1	ILE	1529	-4.200	12.344	7.843	1.00	29.52

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ATOM	519	CD1	ILE	1529	-5.143	13.308	7.133	1.00	32.07
ATOM	520	C	ILE	1529	-1.698	9.608	6.768	1.00	31.50
ATOM	521	O	ILE	1529	-2.009	8.419	6.780	1.00	30.75
ATOM	522	N	SER	1530	-0.749	10.100	5.974	1.00	33.28
ATOM	524	CA	SER	1530	-0.011	9.250	5.038	1.00	32.48
ATOM	525	CB	SER	1530	1.114	10.042	4.368	1.00	37.20
ATOM	526	OG	SER	1530	0.604	11.218	3.766	1.00	49.93
ATOM	528	C	SER	1530	0.583	8.045	5.756	1.00	29.05
ATOM	529	O	SER	1530	0.397	6.909	5.316	1.00	28.66
ATOM	530	N	GLU	1531	1.259	8.290	6.878	1.00	28.21
ATOM	532	CA	GLU	1531	1.880	7.207	7.631	1.00	27.30
ATOM	533	CB	GLU	1531	2.656	7.733	8.839	1.00	28.90
ATOM	534	CG	GLU	1531	3.271	6.609	9.672	1.00	27.17
ATOM	535	CD	GLU	1531	4.047	7.081	10.886	1.00	30.07
ATOM	536	OE1	GLU	1531	4.779	6.244	11.448	1.00	34.78
ATOM	537	OE2	GLU	1531	3.931	8.256	11.291	1.00	31.96
ATOM	538	C	GLU	1531	0.870	6.162	8.072	1.00	27.73
ATOM	539	O	GLU	1531	1.160	4.961	8.028	1.00	28.72
ATOM	540	N	MET	1532	-0.286	6.621	8.555	1.00	29.78
ATOM	542	CA	MET	1532	-1.373	5.734	8.990	1.00	28.79
ATOM	543	CB	MET	1532	-2.501	6.553	9.646	1.00	28.90
ATOM	544	CG	MET	1532	-3.763	5.741	9.993	1.00	29.73
ATOM	545	SD	MET	1532	-5.089	6.693	10.765	1.00	30.19
ATOM	546	CE	MET	1532	-5.455	7.870	9.494	1.00	26.70
ATOM	547	C	MET	1532	-1.935	4.937	7.796	1.00	28.34
ATOM	548	O	MET	1532	-2.166	3.730	7.893	1.00	26.62
ATOM	549	N	GLU	1533	-2.165	5.624	6.678	1.00	28.85
ATOM	551	CA	GLU	1533	-2.684	4.984	5.467	1.00	28.24
ATOM	552	CB	GLU	1533	-2.936	6.027	4.384	1.00	25.42
ATOM	553	CG	GLU	1533	-4.099	6.956	4.719	1.00	30.05
ATOM	554	CD	GLU	1533	-5.393	6.201	5.021	1.00	29.47
ATOM	555	OE1	GLU	1533	-5.794	5.336	4.211	1.00	29.01
ATOM	556	OE2	GLU	1533	-6.011	6.472	6.073	1.00	33.98
ATOM	557	C	GLU	1533	-1.694	3.944	4.968	1.00	28.01
ATOM	558	O	GLU	1533	-2.072	2.845	4.573	1.00	27.39
ATOM	559	N	MET	1534	-0.416	4.293	5.036	1.00	29.06
ATOM	561	CA	MET	1534	0.662	3.413	4.621	1.00	29.74
ATOM	562	CB	MET	1534	1.992	4.155	4.755	1.00	33.16
ATOM	563	CG	MET	1534	3.198	3.270	4.682	1.00	42.88
ATOM	564	SD	MET	1534	3.805	3.127	3.042	1.00	50.20
ATOM	565	CE	MET	1534	5.137	4.169	3.159	1.00	42.64
ATOM	566	C	MET	1534	0.641	2.156	5.493	1.00	26.90
ATOM	567	O	MET	1534	0.755	1.038	4.990	1.00	27.05
ATOM	568	N	MET	1535	0.512	2.348	6.803	1.00	25.42
ATOM	570	CA	MET	1535	0.437	1.233	7.737	1.00	25.88
ATOM	571	CB	MET	1535	0.325	1.741	9.181	1.00	27.63
ATOM	572	CG	MET	1535	1.607	2.391	9.737	1.00	27.26
ATOM	573	SD	MET	1535	1.584	2.561	11.564	1.00	29.49
ATOM	574	CE	MET	1535	1.294	4.255	11.699	1.00	28.22
ATOM	575	C	MET	1535	-0.754	0.324	7.396	1.00	26.28
ATOM	576	O	MET	1535	-0.645	-0.908	7.469	1.00	25.93
ATOM	577	N	LYS	1536	-1.890	0.928	7.032	1.00	27.19
ATOM	579	CA	LYS	1536	-3.087	0.162	6.647	1.00	27.20
ATOM	580	CB	LYS	1536	-4.257	1.088	6.310	1.00	25.29

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ATOM	581	CG	LYS	1536	-4.897	1.770	7.491	1.00	23.86
ATOM	582	CD	LYS	1536	-5.884	2.820	7.017	1.00	22.16
ATOM	583	CE	LYS	1536	-6.460	3.588	8.174	1.00	22.25
ATOM	584	NZ	LYS	1536	-7.484	4.541	7.713	1.00	23.40
ATOM	588	C	LYS	1536	-2.785	-0.699	5.423	1.00	24.52
ATOM	589	O	LYS	1536	-3.069	-1.889	5.403	1.00	26.61
ATOM	590	N	MET	1537	-2.183	-0.093	4.411	1.00	27.12
ATOM	592	CA	MET	1537	-1.843	-0.815	3.194	1.00	28.06
ATOM	593	CB	MET	1537	-1.269	0.147	2.147	1.00	30.36
ATOM	594	CG	MET	1537	-2.265	1.164	1.591	1.00	36.31
ATOM	595	SD	MET	1537	-3.699	0.444	0.727	1.00	42.19
ATOM	596	CE	MET	1537	-2.912	-0.057	-0.793	1.00	36.22
ATOM	597	C	MET	1537	-0.857	-1.952	3.447	1.00	26.98
ATOM	598	O	MET	1537	-1.060	-3.065	2.963	1.00	25.34
ATOM	599	N	ILE	1538	0.188	-1.678	4.229	1.00	27.69
ATOM	601	CA	ILE	1538	1.234	-2.674	4.535	1.00	25.39
ATOM	602	CB	ILE	1538	2.454	-2.006	5.255	1.00	24.42
ATOM	603	CG2	ILE	1538	3.424	-3.051	5.811	1.00	25.28
ATOM	604	CG1	ILE	1538	3.223	-1.131	4.269	1.00	23.88
ATOM	605	CD1	ILE	1538	4.373	-0.372	4.901	1.00	27.19
ATOM	606	C	ILE	1538	0.760	-3.922	5.292	1.00	25.59
ATOM	607	O	ILE	1538	1.242	-5.033	5.035	1.00	26.11
ATOM	608	N	GLY	1539	-0.193	-3.767	6.208	1.00	26.13
ATOM	610	CA	GLY	1539	-0.661	-4.940	6.934	1.00	25.25
ATOM	611	C	GLY	1539	0.191	-5.280	8.149	1.00	26.77
ATOM	612	O	GLY	1539	1.214	-4.637	8.414	1.00	25.42
ATOM	613	N	LYS	1540	-0.204	-6.327	8.862	1.00	25.62
ATOM	615	CA	LYS	1540	0.467	-6.716	10.092	1.00	26.38
ATOM	616	CB	LYS	1540	-0.552	-7.283	11.084	1.00	27.15
ATOM	617	CG	LYS	1540	-1.573	-6.303	11.550	1.00	34.23
ATOM	618	CD	LYS	1540	-2.528	-6.943	12.546	1.00	40.69
ATOM	619	CE	LYS	1540	-3.559	-5.927	13.057	1.00	44.08
ATOM	620	NZ	LYS	1540	-2.956	-4.800	13.833	1.00	44.05
ATOM	624	C	LYS	1540	1.609	-7.705	10.014	1.00	24.37
ATOM	625	O	LYS	1540	1.627	-8.600	9.181	1.00	26.12
ATOM	626	N	HIS	1541	2.545	-7.538	10.936	1.00	24.41
ATOM	628	CA	HIS	1541	3.666	-8.440	11.091	1.00	25.41
ATOM	629	CB	HIS	1541	4.772	-8.228	10.057	1.00	21.88
ATOM	630	CG	HIS	1541	5.798	-9.320	10.068	1.00	22.68
ATOM	631	CD2	HIS	1541	5.823	-10.522	9.444	1.00	21.40
ATOM	632	ND1	HIS	1541	6.939	-9.268	10.843	1.00	22.12
ATOM	634	CE1	HIS	1541	7.619	-10.389	10.697	1.00	24.78
ATOM	635	NE2	HIS	1541	6.966	-11.167	9.854	1.00	27.00
ATOM	637	C	HIS	1541	4.234	-8.328	12.494	1.00	25.47
ATOM	638	O	HIS	1541	4.364	-7.239	13.050	1.00	26.77
ATOM	639	N	LYS	1542	4.560	-9.476	13.063	1.00	26.38
ATOM	641	CA	LYS	1542	5.127	-9.552	14.401	1.00	30.07
ATOM	642	CB	LYS	1542	5.515	-11.003	14.692	1.00	31.38
ATOM	643	CG	LYS	1542	6.061	-11.252	16.077	1.00	42.79
ATOM	644	CD	LYS	1542	6.289	-12.735	16.294	1.00	50.84
ATOM	645	CE	LYS	1542	7.041	-13.374	15.114	1.00	56.75
ATOM	646	NZ	LYS	1542	7.511	-14.763	15.424	1.00	61.29
ATOM	650	C	LYS	1542	6.342	-8.652	14.624	1.00	27.65
ATOM	651	O	LYS	1542	6.519	-8.113	15.711	1.00	26.83

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ATOM	652	N	ASN	1543	7.146	-8.445	13.585	1.00	27.20
ATOM	654	CA	ASN	1543	8.354	-7.642	13.735	1.00	25.50
ATOM	655	CB	ASN	1543	9.578	-8.431	13.260	1.00	25.59
ATOM	656	CG	ASN	1543	9.712	-9.767	13.974	1.00	22.64
ATOM	657	OD1	ASN	1543	9.522	-10.821	13.371	1.00	26.76
ATOM	658	ND2	ASN	1543	9.970	-9.727	15.273	1.00	25.56
ATOM	661	C	ASN	1543	8.374	-6.213	13.226	1.00	25.48
ATOM	662	O	ASN	1543	9.417	-5.692	12.842	1.00	24.58
ATOM	663	N	ILE	1544	7.209	-5.575	13.244	1.00	24.60
ATOM	665	CA	ILE	1544	7.065	-4.177	12.868	1.00	22.32
ATOM	666	CB	ILE	1544	6.524	-3.972	11.409	1.00	25.82
ATOM	667	CG2	ILE	1544	7.401	-4.720	10.403	1.00	24.24
ATOM	668	CG1	ILE	1544	5.057	-4.411	11.279	1.00	26.04
ATOM	669	CD1	ILE	1544	4.446	-4.121	9.901	1.00	23.20
ATOM	670	C	ILE	1544	6.075	-3.598	13.881	1.00	22.37
ATOM	671	O	ILE	1544	5.364	-4.345	14.559	1.00	21.68
ATOM	672	N	ILE	1545	6.111	-2.290	14.076	1.00	23.72
ATOM	674	CA	ILE	1545	5.169	-1.650	14.989	1.00	25.92
ATOM	675	CB	ILE	1545	5.602	-0.199	15.364	1.00	27.24
ATOM	676	CG2	ILE	1545	4.452	0.554	16.035	1.00	22.76
ATOM	677	CG1	ILE	1545	6.839	-0.219	16.285	1.00	25.57
ATOM	678	CD1	ILE	1545	6.591	-0.797	17.686	1.00	24.66
ATOM	679	C	ILE	1545	3.877	-1.612	14.179	1.00	26.03
ATOM	680	O	ILE	1545	3.823	-0.988	13.122	1.00	25.70
ATOM	681	N	ASN	1546	2.849	-2.293	14.669	1.00	24.79
ATOM	683	CA	ASN	1546	1.577	-2.354	13.956	1.00	25.51
ATOM	684	CB	ASN	1546	0.922	-3.727	14.137	1.00	25.17
ATOM	685	CG	ASN	1546	1.730	-4.839	13.539	1.00	21.67
ATOM	686	OD1	ASN	1546	1.856	-4.947	12.329	1.00	24.29
ATOM	687	ND2	ASN	1546	2.278	-5.686	14.384	1.00	22.24
ATOM	690	C	ASN	1546	0.578	-1.276	14.349	1.00	26.85
ATOM	691	O	ASN	1546	0.630	-0.724	15.453	1.00	28.67
ATOM	692	N	LEU	1547	-0.301	-0.956	13.407	1.00	27.70
ATOM	694	CA	LEU	1547	-1.357	0.019	13.622	1.00	27.64
ATOM	695	CB	LEU	1547	-1.945	0.481	12.284	1.00	24.87
ATOM	696	CG	LEU	1547	-3.173	1.400	12.337	1.00	23.25
ATOM	697	CD1	LEU	1547	-2.790	2.763	12.929	1.00	23.76
ATOM	698	CD2	LEU	1547	-3.757	1.569	10.923	1.00	23.47
ATOM	699	C	LEU	1547	-2.415	-0.771	14.396	1.00	27.27
ATOM	700	O	LEU	1547	-2.663	-1.952	14.103	1.00	25.27
ATOM	701	N	LEU	1548	-3.000	-0.130	15.400	1.00	27.94
ATOM	703	CA	LEU	1548	-4.017	-0.770	16.223	1.00	26.98
ATOM	704	CB	LEU	1548	-3.623	-0.735	17.708	1.00	24.65
ATOM	705	CG	LEU	1548	-2.327	-1.450	18.108	1.00	25.38
ATOM	706	CD1	LEU	1548	-2.189	-1.428	19.613	1.00	25.73
ATOM	707	CD2	LEU	1548	-2.337	-2.886	17.621	1.00	23.92
ATOM	708	C	LEU	1548	-5.369	-0.113	16.042	1.00	26.65
ATOM	709	O	LEU	1548	-6.392	-0.752	16.238	1.00	27.11
ATOM	710	N	GLY	1549	-5.378	1.163	15.684	1.00	25.04
ATOM	712	CA	GLY	1549	-6.643	1.855	15.516	1.00	25.47
ATOM	713	C	GLY	1549	-6.417	3.336	15.367	1.00	26.23
ATOM	714	O	GLY	1549	-5.267	3.781	15.287	1.00	28.41
ATOM	715	N	ALA	1550	-7.501	4.104	15.349	1.00	25.49
ATOM	717	CA	ALA	1550	-7.408	5.550	15.198	1.00	24.81

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ATOM	718	CB	ALA	1550	-7.176	5.913	13.724	1.00	21.79
ATOM	719	C	ALA	1550	-8.645	6.271	15.691	1.00	25.51
ATOM	720	O	ALA	1550	-9.738	5.702	15.726	1.00	24.09
ATOM	721	N	CYS	1551	-8.440	7.527	16.080	1.00	24.90
ATOM	724	CA	CYS	1551	-9.492	8.438	16.511	1.00	26.80
ATOM	725	SG	CYS	1551	-9.243	8.932	17.944	1.00	26.32
ATOM	726	C	CYS	1551	-9.333	7.655	19.223	1.00	32.31
ATOM	727	O	CYS	1551	-9.341	9.585	15.502	1.00	28.31
ATOM	728	N	THR	1552	-8.361	10.338	15.537	1.00	28.42
ATOM	730	CA	THR	1552	-10.261	9.660	14.547	1.00	28.38
ATOM	731	CB	THR	1552	-10.198	10.671	13.498	1.00	31.26
ATOM	732	OG1	THR	1552	-10.159	9.977	12.095	1.00	30.07
ATOM	734	CG2	THR	1552	-11.406	9.309	11.836	1.00	29.64
ATOM	735	C	THR	1552	-9.044	8.945	12.053	1.00	28.65
ATOM	736	O	THR	1552	-11.355	11.662	13.509	1.00	33.31
ATOM	737	N	GLN	1553	-11.295	12.722	12.874	1.00	31.94
ATOM	739	CA	GLN	1553	-12.420	11.309	14.214	1.00	36.09
ATOM	740	CB	GLN	1553	-13.598	12.158	14.245	1.00	39.26
ATOM	741	CG	GLN	1553	-14.864	11.299	14.145	1.00	36.61
ATOM	742	CD	GLN	1553	-14.932	10.436	12.881	1.00	37.72
ATOM	743	OE1	GLN	1553	-14.762	11.247	11.601	1.00	38.41
ATOM	744	NE2	GLN	1553	-15.491	12.210	11.363	1.00	37.88
ATOM	747	C	GLN	1553	-13.798	10.858	10.770	1.00	37.67
ATOM	748	O	GLN	1553	-13.671	13.079	15.451	1.00	41.28
ATOM	749	N	ASP	1554	-13.150	12.758	16.513	1.00	41.37
ATOM	751	CA	ASP	1554	-14.282	14.246	15.243	1.00	44.93
ATOM	752	CB	ASP	1554	-14.487	15.254	16.281	1.00	48.05
ATOM	753	CG	ASP	1554	-15.828	15.009	16.975	1.00	50.80
ATOM	754	OD1	ASP	1554	-17.007	15.281	16.067	1.00	56.88
ATOM	755	OD2	ASP	1554	-17.921	16.019	16.491	1.00	63.89
ATOM	756	C	ASP	1554	-17.016	14.776	14.925	1.00	58.98
ATOM	757	O	ASP	1554	-13.367	15.366	17.316	1.00	48.04
ATOM	758	N	GLY	1555	-13.556	15.056	18.502	1.00	48.73
ATOM	760	CA	GLY	1555	-12.205	15.819	16.860	1.00	44.30
ATOM	761	C	GLY	1555	-11.080	15.960	17.756	1.00	42.32
ATOM	762	O	GLY	1555	-9.761	15.713	17.052	1.00	40.69
ATOM	763	N	PRO	1556	-9.740	15.465	15.848	1.00	40.71
ATOM	764	CD	PRO	1556	-8.644	15.776	17.782	1.00	39.49
ATOM	765	CA	PRO	1556	-8.585	15.983	19.235	1.00	40.36
ATOM	766	CB	PRO	1556	-7.298	15.566	17.250	1.00	38.37
ATOM	767	CG	PRO	1556	-6.405	15.771	18.470	1.00	38.47
ATOM	768	C	PRO	1556	-7.226	16.573	19.388	1.00	41.77
ATOM	769	O	PRO	1556	-7.140	14.154	16.746	1.00	36.92
ATOM	770	N	LEU	1557	-7.606	13.208	17.371	1.00	37.04
ATOM	772	CA	LEU	1557	-6.447	14.017	15.627	1.00	36.70
ATOM	773	CB	LEU	1557	-6.201	12.719	15.037	1.00	34.81
ATOM	774	CG	LEU	1557	-5.528	12.885	13.664	1.00	32.49
ATOM	775	CD1	LEU	1557	-5.004	11.623	12.954	1.00	30.83
ATOM	776	CD2	LEU	1557	-6.146	10.655	12.664	1.00	26.28
ATOM	777	C	LEU	1557	-4.283	12.014	11.672	1.00	25.55
ATOM	778	O	LEU	1557	-5.290	11.925	15.961	1.00	33.63
ATOM	779	N	TYR	1558	-4.229	12.410	16.369	1.00	33.62
ATOM	781	CA	TYR	1558	-5.718	10.724	16.319	1.00	31.97
					-4.902	9.863	17.147	1.00	31.81

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ATOM	782	CB	TYR	1558	-5.614	9.500	18.462	1.00	33.55
ATOM	783	CG	TYR	1558	-5.710	10.638	19.461	1.00	35.33
ATOM	784	CD1	TYR	1558	-6.644	10.608	20.499	1.00	35.68
ATOM	785	CE1	TYR	1558	-6.757	11.670	21.394	1.00	38.60
ATOM	786	CD2	TYR	1558	-4.883	11.759	19.349	1.00	38.62
ATOM	787	CE2	TYR	1558	-4.985	12.824	20.235	1.00	40.33
ATOM	788	CZ	TYR	1558	-5.924	12.781	21.254	1.00	41.70
ATOM	789	OH	TYR	1558	-6.040	13.867	22.104	1.00	42.66
ATOM	791	C	TYR	1558	-4.607	8.604	16.345	1.00	31.08
ATOM	792	O	TYR	1558	-5.527	7.937	15.857	1.00	31.28
ATOM	793	N	VAL	1559	-3.328	8.336	16.116	1.00	28.34
ATOM	795	CA	VAL	1559	-2.934	7.132	15.403	1.00	26.39
ATOM	796	CB	VAL	1559	-1.830	7.401	14.364	1.00	29.17
ATOM	797	CG1	VAL	1559	-1.463	6.103	13.648	1.00	26.25
ATOM	798	CG2	VAL	1559	-2.297	8.461	13.360	1.00	29.56
ATOM	799	C	VAL	1559	-2.411	6.226	16.498	1.00	25.14
ATOM	800	O	VAL	1559	-1.396	6.522	17.120	1.00	28.04
ATOM	801	N	ILE	1560	-3.164	5.171	16.783	1.00	25.28
ATOM	803	CA	ILE	1560	-2.832	4.208	17.831	1.00	24.81
ATOM	804	CB	ILE	1560	-4.133	3.669	18.496	1.00	24.63
ATOM	805	CG2	ILE	1560	-3.790	2.812	19.728	1.00	20.93
ATOM	806	CG1	ILE	1560	-5.044	4.854	18.869	1.00	22.94
ATOM	807	CD1	ILE	1560	-6.499	4.502	19.028	1.00	25.34
ATOM	808	C	ILE	1560	-1.994	3.051	17.286	1.00	26.38
ATOM	809	O	ILE	1560	-2.429	2.301	16.398	1.00	26.14
ATOM	810	N	VAL	1561	-0.782	2.911	17.809	1.00	27.31
ATOM	812	CA	VAL	1561	0.112	1.852	17.359	1.00	27.32
ATOM	813	CB	VAL	1561	1.309	2.435	16.527	1.00	25.01
ATOM	814	CG1	VAL	1561	0.785	3.220	15.338	1.00	19.39
ATOM	815	CG2	VAL	1561	2.170	3.340	17.397	1.00	26.08
ATOM	816	C	VAL	1561	0.615	1.029	18.548	1.00	25.89
ATOM	817	O	VAL	1561	0.364	1.373	19.713	1.00	25.64
ATOM	818	N	GLU	1562	1.288	-0.076	18.250	1.00	24.49
ATOM	820	CA	GLU	1562	1.806	-0.949	19.284	1.00	25.00
ATOM	821	CB	GLU	1562	2.357	-2.231	18.677	1.00	23.69
ATOM	822	CG	GLU	1562	1.272	-3.170	18.219	1.00	24.29
ATOM	823	CD	GLU	1562	1.814	-4.393	17.514	1.00	27.65
ATOM	824	OE1	GLU	1562	1.218	-5.480	17.649	1.00	29.50
ATOM	825	OE2	GLU	1562	2.832	-4.270	16.807	1.00	32.34
ATOM	826	C	GLU	1562	2.840	-0.279	20.170	1.00	27.27
ATOM	827	O	GLU	1562	3.596	0.576	19.729	1.00	26.18
ATOM	828	N	TYR	1563	2.822	-0.663	21.441	1.00	30.39
ATOM	830	CA	TYR	1563	3.715	-0.121	22.454	1.00	32.48
ATOM	831	CB	TYR	1563	2.932	0.132	23.750	1.00	33.91
ATOM	832	CG	TYR	1563	3.788	0.535	24.928	1.00	34.93
ATOM	833	CD1	TYR	1563	4.606	1.664	24.871	1.00	34.50
ATOM	834	CE1	TYR	1563	5.374	2.051	25.967	1.00	37.77
ATOM	835	CD2	TYR	1563	3.758	-0.201	26.108	1.00	33.54
ATOM	836	CE2	TYR	1563	4.519	0.171	27.205	1.00	34.94
ATOM	837	CZ	TYR	1563	5.321	1.296	27.128	1.00	37.22
ATOM	838	OH	TYR	1563	6.087	1.648	28.206	1.00	45.36
ATOM	840	C	TYR	1563	4.896	-1.039	22.730	1.00	31.53
ATOM	841	O	TYR	1563	4.737	-2.252	22.895	1.00	30.43
ATOM	842	N	ALA	1564	6.082	-0.444	22.761	1.00	32.28

ATOM	844	CA	ALA	1564	7.326	-1.167	23.026	1.00	32.59
ATOM	845	CB	ALA	1564	8.308	-0.957	21.863	1.00	30.11
ATOM	846	C	ALA	1564	7.897	-0.608	24.334	1.00	31.81
ATOM	847	O	ALA	1564	8.563	0.427	24.345	1.00	34.11
ATOM	848	N	SER	1565	7.619	-1.296	25.434	1.00	34.09
ATOM	850	CA	SER	1565	8.039	-0.853	26.763	1.00	35.05
ATOM	851	CB	SER	1565	7.400	-1.725	27.829	1.00	30.13
ATOM	852	OG	SER	1565	7.689	-3.084	27.579	1.00	38.17
ATOM	854	C	SER	1565	9.526	-0.769	27.041	1.00	35.03
ATOM	855	O	SER	1565	9.947	-0.001	27.902	1.00	37.12
ATOM	856	N	LYS	1566	10.321	-1.557	26.330	1.00	34.55
ATOM	858	CA	LYS	1566	11.756	-1.559	26.562	1.00	33.48
ATOM	859	CB	LYS	1566	12.291	-2.990	26.508	1.00	31.90
ATOM	860	CG	LYS	1566	11.674	-3.865	27.586	1.00	28.63
ATOM	861	CD	LYS	1566	12.162	-5.287	27.508	1.00	34.97
ATOM	862	CE	LYS	1566	11.763	-6.042	28.761	1.00	36.82
ATOM	863	NZ	LYS	1566	12.288	-7.433	28.748	1.00	41.32
ATOM	867	C	LYS	1566	12.567	-0.613	25.691	1.00	34.98
ATOM	868	O	LYS	1566	13.785	-0.740	25.607	1.00	38.03
ATOM	869	N	GLY	1567	11.892	0.338	25.049	1.00	36.00
ATOM	871	CA	GLY	1567	12.582	1.322	24.222	1.00	34.14
ATOM	872	C	GLY	1567	13.245	0.864	22.933	1.00	32.01
ATOM	873	O	GLY	1567	12.975	-0.222	22.439	1.00	31.95
ATOM	874	N	ASN	1568	14.091	1.719	22.360	1.00	33.51
ATOM	876	CA	ASN	1568	14.774	1.375	21.121	1.00	34.20
ATOM	877	CB	ASN	1568	15.203	2.627	20.332	1.00	34.07
ATOM	878	CG	ASN	1568	16.420	3.321	20.910	1.00	35.09
ATOM	879	OD1	ASN	1568	17.453	2.709	21.156	1.00	34.36
ATOM	880	ND2	ASN	1568	16.317	4.624	21.066	1.00	38.38
ATOM	883	C	ASN	1568	15.927	0.401	21.325	1.00	33.38
ATOM	884	O	ASN	1568	16.490	0.315	22.414	1.00	34.93
ATOM	885	N	LEU	1569	16.276	-0.317	20.263	1.00	31.11
ATOM	887	CA	LEU	1569	17.333	-1.316	20.298	1.00	30.44
ATOM	888	CB	LEU	1569	17.437	-2.008	18.928	1.00	29.46
ATOM	889	CG	LEU	1569	18.438	-3.148	18.741	1.00	29.01
ATOM	890	CD1	LEU	1569	18.285	-4.219	19.840	1.00	28.81
ATOM	891	CD2	LEU	1569	18.263	-3.740	17.338	1.00	26.62
ATOM	892	C	LEU	1569	18.706	-0.805	20.762	1.00	30.16
ATOM	893	O	LEU	1569	19.400	-1.501	21.496	1.00	27.32
ATOM	894	N	ARG	1570	19.097	0.396	20.344	1.00	30.74
ATOM	896	CA	ARG	1570	20.386	0.951	20.758	1.00	33.72
ATOM	897	CB	ARG	1570	20.597	2.349	20.160	1.00	32.82
ATOM	898	CG	ARG	1570	21.873	3.009	20.662	1.00	36.90
ATOM	899	CD	ARG	1570	21.966	4.481	20.332	1.00	39.32
ATOM	900	NE	ARG	1570	20.749	5.222	20.664	1.00	50.32
ATOM	902	CZ	ARG	1570	20.376	5.600	21.889	1.00	51.90
ATOM	903	NH1	ARG	1570	21.118	5.316	22.960	1.00	50.15
ATOM	906	NH2	ARG	1570	19.246	6.284	22.033	1.00	53.67
ATOM	909	C	ARG	1570	20.434	1.022	22.298	1.00	35.75
ATOM	910	O	ARG	1570	21.324	0.444	22.939	1.00	35.67
ATOM	911	N	GLU	1571	19.444	1.695	22.880	1.00	35.56
ATOM	913	CA	GLU	1571	19.331	1.835	24.328	1.00	36.50
ATOM	914	CB	GLU	1571	18.055	2.607	24.667	1.00	39.08
ATOM	915	CG	GLU	1571	18.061	4.056	24.208	1.00	46.75

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ATOM	916	CD	GLU	1571	16.694	4.721	24.311	1.00	51.36
ATOM	917	OE1	GLU	1571	15.676	3.996	24.417	1.00	55.22
ATOM	918	OE2	GLU	1571	16.635	5.972	24.267	1.00	53.59
ATOM	919	C	GLU	1571	19.314	0.469	25.022	1.00	34.82
ATOM	920	O	GLU	1571	20.018	0.242	26.013	1.00	35.05
ATOM	921	N	TYR	1572	18.520	-0.441	24.469	1.00	33.35
ATOM	923	CA	TYR	1572	18.366	-1.796	24.986	1.00	31.83
ATOM	924	CB	TYR	1572	17.365	-2.544	24.102	1.00	30.77
ATOM	925	CG	TYR	1572	17.170	-4.008	24.408	1.00	28.50
ATOM	926	CD1	TYR	1572	16.193	-4.420	25.313	1.00	30.48
ATOM	927	CE1	TYR	1572	15.977	-5.760	25.574	1.00	30.97
ATOM	928	CD2	TYR	1572	17.933	-4.985	23.772	1.00	26.14
ATOM	929	CE2	TYR	1572	17.725	-6.329	24.027	1.00	26.21
ATOM	930	CZ	TYR	1572	17.725	-6.708	24.935	1.00	30.30
ATOM	931	OH	TYR	1572	16.742	-6.708	24.935	1.00	33.52
ATOM	933	C	TYR	1572	16.518	-8.041	25.214	1.00	34.83
ATOM	934	O	TYR	1572	19.692	-2.556	25.044	1.00	34.93
ATOM	935	N	LEU	1573	19.959	-3.308	25.992	1.00	34.93
ATOM	937	CA	LEU	1573	20.517	-2.370	24.020	1.00	34.34
ATOM	938	CB	LEU	1573	21.803	-3.053	23.961	1.00	35.38
ATOM	939	CG	LEU	1573	22.357	-3.027	22.531	1.00	32.71
ATOM	940	CD1	LEU	1573	21.669	-3.891	21.464	1.00	29.16
ATOM	941	CD2	LEU	1573	22.161	-3.503	20.087	1.00	26.98
ATOM	942	C	LEU	1573	21.932	-5.351	21.710	1.00	28.85
ATOM	943	O	LEU	1573	22.799	-2.420	24.933	1.00	37.54
ATOM	944	N	GLN	1574	23.511	-3.123	25.659	1.00	36.67
ATOM	946	CA	GLN	1574	22.814	-1.092	24.969	1.00	37.90
ATOM	947	CB	GLN	1574	23.729	-0.368	25.838	1.00	39.77
ATOM	948	CG	GLN	1574	23.624	1.138	25.572	1.00	40.09
ATOM	949	CD	GLN	1574	24.208	1.549	24.217	1.00	42.28
ATOM	950	OE1	GLN	1574	24.030	3.018	23.896	1.00	44.28
ATOM	951	NE2	GLN	1574	23.362	3.755	24.615	1.00	47.55
ATOM	954	C	GLN	1574	24.613	3.448	22.790	1.00	46.09
ATOM	955	O	GLN	1574	23.490	-0.697	27.310	1.00	40.75
ATOM	956	N	ALA	1575	24.440	-0.939	28.059	1.00	41.29
ATOM	958	CA	ALA	1575	22.220	-0.783	27.696	1.00	40.10
ATOM	959	CB	ALA	1575	21.842	-1.088	29.069	1.00	38.81
ATOM	960	C	ALA	1575	20.349	-0.819	29.273	1.00	35.69
ATOM	961	O	ALA	1575	22.192	-2.514	29.503	1.00	40.63
ATOM	962	N	ARG	1576	22.098	-2.843	30.690	1.00	43.39
ATOM	964	CA	ARG	1576	22.602	-3.357	28.561	1.00	38.39
ATOM	965	CB	ARG	1576	22.945	-4.729	28.896	1.00	37.69
ATOM	966	CG	ARG	1576	22.034	-5.689	28.137	1.00	38.16
ATOM	967	CD	ARG	1576	20.594	-5.547	28.589	1.00	37.89
ATOM	968	NE	ARG	1576	19.622	-6.281	27.711	1.00	37.36
ATOM	970	CZ	ARG	1576	18.267	-6.255	28.265	1.00	34.99
ATOM	971	NH1	ARG	1576	17.565	-5.150	28.484	1.00	36.94
ATOM	974	NH2	ARG	1576	18.083	-3.960	28.209	1.00	36.18
ATOM	977	C	ARG	1576	16.310	-5.237	28.909	1.00	40.93
ATOM	978	O	ARG	1576	24.413	-5.073	28.704	1.00	38.93
ATOM	979	N	ARG	1577	24.801	-6.249	28.699	1.00	39.75
ATOM	981	CA	ARG	1577	25.233	-4.036	28.570	1.00	39.21
ATOM	982	CB	ARG	1577	26.671	-4.196	28.413	1.00	38.97
ATOM	983	CG	ARG	1577	27.307	-2.870	28.000	1.00	36.06
					26.992	-2.408	26.610	1.00	36.41

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ATOM	984	CD	ARG	1577	27.695	-1.094	26.337	1.00	36.17
ATOM	985	NE	ARG	1577	27.776	-0.806	24.907	1.00	38.45
ATOM	987	CZ	ARG	1577	28.284	0.309	24.387	1.00	39.00
ATOM	988	NH1	ARG	1577	28.764	1.262	25.175	1.00	38.88
ATOM	991	NH2	ARG	1577	28.311	0.469	23.071	1.00	37.76
ATOM	994	C	ARG	1577	27.247	-4.571	29.772	1.00	40.59
ATOM	995	O	ARG	1577	26.680	-4.217	30.800	1.00	38.52
ATOM	996	N	PRO	1578	28.358	-5.327	29.796	1.00	43.19
ATOM	997	CD	PRO	1578	29.077	-5.980	28.692	1.00	44.84
ATOM	998	CA	PRO	1578	28.952	-5.692	31.088	1.00	45.06
ATOM	999	CB	PRO	1578	30.065	-6.673	30.689	1.00	44.86
ATOM	1000	CG	PRO	1578	30.431	-6.229	29.308	1.00	44.56
ATOM	1001	C	PRO	1578	29.513	-4.420	31.734	1.00	44.93
ATOM	1002	O	PRO	1578	29.809	-3.439	31.043	1.00	43.13
ATOM	1003	N	PRO	1579	29.649	-4.414	33.067	1.00	47.61
ATOM	1004	CD	PRO	1579	29.315	-5.492	34.012	1.00	48.39
ATOM	1005	CA	PRO	1579	30.173	-3.247	33.784	1.00	48.74
ATOM	1006	CB	PRO	1579	30.138	-3.706	35.238	1.00	49.73
ATOM	1007	CG	PRO	1579	29.027	-4.711	35.259	1.00	49.21
ATOM	1008	C	PRO	1579	31.591	-2.888	33.357	1.00	49.67
ATOM	1009	O	PRO	1579	32.483	-3.733	33.361	1.00	52.07
ATOM	1010	N	GLU	1592	19.165	-5.411	32.444	1.00	64.83
ATOM	1012	CA	GLU	1592	20.603	-5.147	32.491	1.00	64.82
ATOM	1013	CB	GLU	1592	20.969	-4.421	33.784	1.00	67.61
ATOM	1014	C	GLU	1592	21.448	-6.413	32.335	1.00	63.99
ATOM	1015	O	GLU	1592	22.653	-6.336	32.098	1.00	65.67
ATOM	1016	N	GLU	1593	20.821	-7.575	32.485	1.00	62.41
ATOM	1018	CA	GLU	1593	21.534	-8.844	32.342	1.00	61.23
ATOM	1019	CB	GLU	1593	20.595	-10.017	32.600	1.00	61.20
ATOM	1020	C	GLU	1593	22.141	-8.953	30.944	1.00	59.26
ATOM	1021	O	GLU	1593	21.494	-8.631	29.945	1.00	59.84
ATOM	1022	N	GLN	1594	23.388	-9.405	30.888	1.00	57.94
ATOM	1024	CA	GLN	1594	24.101	-9.558	29.625	1.00	54.91
ATOM	1025	CB	GLN	1594	25.501	-10.141	29.865	1.00	55.13
ATOM	1026	CG	GLN	1594	26.439	-9.252	30.679	1.00	56.93
ATOM	1027	CD	GLN	1594	27.682	-9.997	31.180	1.00	59.60
ATOM	1028	OE1	GLN	1594	28.241	-10.858	30.488	1.00	58.45
ATOM	1029	NE2	GLN	1594	28.117	-9.662	32.393	1.00	58.95
ATOM	1032	C	GLN	1594	23.331	-10.438	28.640	1.00	52.30
ATOM	1033	O	GLN	1594	22.637	-11.389	29.025	1.00	52.03
ATOM	1034	N	LEU	1595	23.438	-10.091	27.366	1.00	49.60
ATOM	1036	CA	LEU	1595	22.782	-10.836	26.308	1.00	45.16
ATOM	1037	CB	LEU	1595	22.459	-9.907	25.135	1.00	41.36
ATOM	1038	CG	LEU	1595	21.463	-8.815	25.523	1.00	39.43
ATOM	1039	CD1	LEU	1595	21.617	-7.583	24.644	1.00	36.21
ATOM	1040	CD2	LEU	1595	20.060	-9.389	25.480	1.00	34.91
ATOM	1041	C	LEU	1595	23.747	-11.900	25.858	1.00	43.30
ATOM	1042	O	LEU	1595	24.953	-11.675	25.841	1.00	43.62
ATOM	1043	N	SER	1596	23.230	-13.081	25.553	1.00	42.92
ATOM	1045	CA	SER	1596	24.085	-14.150	25.077	1.00	41.86
ATOM	1046	CB	SER	1596	23.410	-15.502	25.298	1.00	40.86
ATOM	1047	OG	SER	1596	22.188	-15.596	24.595	1.00	37.88
ATOM	1049	C	SER	1596	24.322	-13.914	23.587	1.00	41.59
ATOM	1050	O	SER	1596	23.657	-13.077	22.966	1.00	41.94

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ATOM	1051	N	SER	1597	25.275	-14.637	23.018	1.00	39.60
ATOM	1053	CA	SER	1597	25.557	-14.518	21.603	1.00	39.74
ATOM	1054	CB	SER	1597	26.729	-15.409	21.223	1.00	41.38
ATOM	1055	OG	SER	1597	27.824	-15.147	22.077	1.00	50.59
ATOM	1057	C	SER	1597	24.315	-14.921	20.818	1.00	38.16
ATOM	1058	O	SER	1597	24.036	-14.353	19.769	1.00	38.03
ATOM	1059	N	LYS	1598	23.560	-15.891	21.327	1.00	36.40
ATOM	1061	CA	LYS	1598	22.362	-16.312	20.634	1.00	35.97
ATOM	1062	CB	LYS	1598	21.791	-17.594	21.228	1.00	36.69
ATOM	1063	CG	LYS	1598	20.989	-18.402	20.198	1.00	40.42
ATOM	1064	CD	LYS	1598	20.164	-19.499	20.838	1.00	40.37
ATOM	1065	CE	LYS	1598	19.792	-20.572	19.829	1.00	46.34
ATOM	1066	NZ	LYS	1598	20.993	-21.338	19.362	1.00	45.29
ATOM	1070	C	LYS	1598	21.324	-15.194	20.696	1.00	37.49
ATOM	1071	O	LYS	1598	20.567	-14.983	19.738	1.00	38.10
ATOM	1072	N	ASP	1599	21.316	-14.458	21.807	1.00	35.21
ATOM	1074	CA	ASP	1599	20.380	-13.352	21.983	1.00	34.02
ATOM	1075	CB	ASP	1599	20.556	-12.686	23.346	1.00	37.78
ATOM	1076	CG	ASP	1599	19.970	-13.493	24.483	1.00	40.05
ATOM	1077	OD1	ASP	1599	20.270	-13.143	25.642	1.00	42.73
ATOM	1078	OD2	ASP	1599	19.204	-14.450	24.235	1.00	42.39
ATOM	1079	C	ASP	1599	20.633	-12.306	20.922	1.00	32.84
ATOM	1080	O	ASP	1599	19.694	-11.779	20.311	1.00	30.59
ATOM	1081	N	LEU	1600	21.912	-11.999	20.724	1.00	31.11
ATOM	1083	CA	LEU	1600	22.323	-10.998	19.744	1.00	32.17
ATOM	1084	CB	LEU	1600	23.823	-10.722	19.875	1.00	32.30
ATOM	1085	CG	LEU	1600	24.275	-10.162	21.235	1.00	31.08
ATOM	1086	CD1	LEU	1600	25.794	-9.931	21.242	1.00	30.59
ATOM	1087	CD2	LEU	1600	23.549	-8.863	21.514	1.00	28.89
ATOM	1088	C	LEU	1600	21.949	-11.390	18.311	1.00	30.77
ATOM	1089	O	LEU	1600	21.352	-10.601	17.574	1.00	29.87
ATOM	1090	N	VAL	1601	22.269	-12.623	17.933	1.00	30.19
ATOM	1092	CA	VAL	1601	21.954	-13.115	16.602	1.00	29.25
ATOM	1093	CB	VAL	1601	22.593	-14.497	16.349	1.00	31.27
ATOM	1094	CG1	VAL	1601	22.355	-14.936	14.914	1.00	31.60
ATOM	1095	CG2	VAL	1601	24.093	-14.434	16.622	1.00	31.91
ATOM	1096	C	VAL	1601	20.438	-13.181	16.405	1.00	29.06
ATOM	1097	O	VAL	1601	19.946	-12.914	15.310	1.00	27.71
ATOM	1098	N	SER	1602	19.702	-13.511	17.468	1.00	29.10
ATOM	1100	CA	SER	1602	18.243	-13.585	17.400	1.00	29.29
ATOM	1101	CB	SER	1602	17.680	-14.189	18.679	1.00	30.81
ATOM	1102	OG	SER	1602	16.266	-14.074	18.692	1.00	35.78
ATOM	1104	C	SER	1602	17.649	-12.199	17.156	1.00	28.98
ATOM	1105	O	SER	1602	16.662	-12.039	16.426	1.00	26.82
ATOM	1106	N	CYS	1603	18.274	-11.202	17.765	1.00	29.06
ATOM	1108	CA	CYS	1603	17.870	-9.823	17.599	1.00	29.22
ATOM	1109	CB	CYS	1603	18.784	-8.943	18.438	1.00	29.66
ATOM	1110	SG	CYS	1603	18.575	-7.212	18.103	0.50	23.69
ATOM	1111	C	CYS	1603	17.988	-9.422	16.112	1.00	29.23
ATOM	1112	O	CYS	1603	17.087	-8.796	15.552	1.00	27.52
ATOM	1113	N	ALA	1604	19.113	-9.778	15.491	1.00	27.87
ATOM	1115	CA	ALA	1604	19.376	-9.484	14.077	1.00	26.37
ATOM	1116	CB	ALA	1604	20.783	-9.941	13.690	1.00	23.88
ATOM	1117	C	ALA	1604	18.349	-10.203	13.223	1.00	25.82

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ATOM	1118	O	ALA	1604	17.788	-9.631	12.289	1.00	25.84
ATOM	1119	N	TYR	1605	18.119	-11.468	13.544	1.00	25.56
ATOM	1121	CA	TYR	1605	17.152	-12.276	12.827	1.00	27.81
ATOM	1122	CB	TYR	1605	17.080	-13.662	13.456	1.00	26.66
ATOM	1123	CG	TYR	1605	15.974	-14.515	12.886	1.00	30.75
ATOM	1124	CD1	TYR	1605	16.111	-15.141	11.640	1.00	30.20
ATOM	1125	CE1	TYR	1605	15.088	-15.944	11.126	1.00	30.03
ATOM	1126	CD2	TYR	1605	14.790	-14.707	13.596	1.00	30.73
ATOM	1127	CE2	TYR	1605	13.775	-15.500	13.097	1.00	30.71
ATOM	1128	CZ	TYR	1605	13.930	-16.117	11.867	1.00	30.93
ATOM	1129	OH	TYR	1605	12.923	-16.928	11.417	1.00	32.31
ATOM	1131	C	TYR	1605	15.748	-11.641	12.775	1.00	26.15
ATOM	1132	O	TYR	1605	15.147	-11.551	11.702	1.00	26.64
ATOM	1133	N	GLN	1606	15.244	-11.200	13.926	1.00	25.48
ATOM	1135	CA	GLN	1606	13.921	-10.581	14.023	1.00	26.86
ATOM	1136	CB	GLN	1606	13.589	-10.269	15.482	1.00	26.83
ATOM	1137	CG	GLN	1606	13.357	-11.508	16.332	1.00	25.84
ATOM	1138	CD	GLN	1606	13.151	-11.167	17.791	1.00	30.86
ATOM	1139	OE1	GLN	1606	12.202	-10.471	18.150	1.00	31.87
ATOM	1140	NE2	GLN	1606	14.056	-11.631	18.640	1.00	31.67
ATOM	1143	C	GLN	1606	13.835	-9.310	13.186	1.00	27.52
ATOM	1144	O	GLN	1606	12.831	-9.058	12.506	1.00	26.05
ATOM	1145	N	VAL	1607	14.904	-8.523	13.216	1.00	26.68
ATOM	1147	CA	VAL	1607	14.963	-7.301	12.435	1.00	25.66
ATOM	1148	CB	VAL	1607	16.225	-6.485	12.787	1.00	28.50
ATOM	1149	CG1	VAL	1607	16.363	-5.274	11.853	1.00	26.04
ATOM	1150	CG2	VAL	1607	16.151	-6.031	14.246	1.00	24.45
ATOM	1151	C	VAL	1607	14.934	-7.641	10.938	1.00	24.89
ATOM	1152	O	VAL	1607	14.184	-7.033	10.177	1.00	25.86
ATOM	1153	N	ALA	1608	15.738	-8.619	10.522	1.00	25.24
ATOM	1155	CA	ALA	1608	15.773	-9.039	9.120	1.00	22.95
ATOM	1156	CB	ALA	1608	16.813	-10.117	8.920	1.00	20.24
ATOM	1157	C	ALA	1608	14.383	-9.541	8.679	1.00	25.71
ATOM	1158	O	ALA	1608	13.963	-9.319	7.532	1.00	27.48
ATOM	1159	N	ARG	1609	13.676	-10.216	9.585	1.00	27.10
ATOM	1161	CA	ARG	1609	12.327	-10.708	9.301	1.00	28.55
ATOM	1162	CB	ARG	1609	11.840	-11.640	10.397	1.00	31.53
ATOM	1163	CG	ARG	1609	12.407	-13.005	10.290	1.00	36.05
ATOM	1164	CD	ARG	1609	11.537	-13.931	11.056	1.00	40.28
ATOM	1165	NE	ARG	1609	10.849	-14.874	10.190	1.00	42.06
ATOM	1167	CZ	ARG	1609	9.974	-15.771	10.632	1.00	42.08
ATOM	1168	NH1	ARG	1609	9.678	-15.834	11.928	1.00	40.32
ATOM	1171	NH2	ARG	1609	9.416	-16.620	9.784	1.00	43.27
ATOM	1174	C	ARG	1609	11.329	-9.569	9.124	1.00	25.55
ATOM	1175	O	ARG	1609	10.469	-9.621	8.231	1.00	26.98
ATOM	1176	N	GLY	1610	11.418	-8.565	9.996	1.00	23.92
ATOM	1178	CA	GLY	1610	10.555	-7.406	9.870	1.00	22.19
ATOM	1179	C	GLY	1610	10.800	-6.747	8.512	1.00	25.92
ATOM	1180	O	GLY	1610	9.855	-6.424	7.772	1.00	23.49
ATOM	1181	N	MET	1611	12.076	-6.589	8.163	1.00	23.15
ATOM	1183	CA	MET	1611	12.456	-5.989	6.888	1.00	22.57
ATOM	1184	CB	MET	1611	13.956	-5.710	6.849	1.00	22.18
ATOM	1185	CG	MET	1611	14.398	-4.542	7.729	1.00	22.63
ATOM	1186	SD	MET	1611	13.478	-3.006	7.426	1.00	25.23

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ATOM	1187	CE	MET	1611	13.812	-2.688	5.675	1.00	21.38
ATOM	1188	C	MET	1611	12.050	-6.848	5.681	1.00	23.96
ATOM	1189	O	MET	1611	11.673	-6.326	4.633	1.00	25.26
ATOM	1190	N	GLU	1612	12.130	-8.163	5.822	1.00	24.34
ATOM	1192	CA	GLU	1612	11.755	-9.043	4.733	1.00	25.56
ATOM	1193	CB	GLU	1612	12.018	-10.494	5.121	1.00	24.96
ATOM	1194	CG	GLU	1612	11.703	-11.488	4.009	1.00	26.79
ATOM	1195	CD	GLU	1612	11.812	-12.931	4.450	1.00	26.96
ATOM	1196	OE1	GLU	1612	11.557	-13.212	5.636	1.00	30.98
ATOM	1197	OE2	GLU	1612	12.154	-13.791	3.611	1.00	32.31
ATOM	1198	C	GLU	1612	10.267	-8.829	4.415	1.00	25.70
ATOM	1199	O	GLU	1612	9.860	-8.753	3.252	1.00	24.30
ATOM	1200	N	TYR	1613	9.463	-8.723	5.465	1.00	23.55
ATOM	1202	CA	TYR	1613	8.037	-8.501	5.294	1.00	22.94
ATOM	1203	CB	TYR	1613	7.314	-8.586	6.650	1.00	24.00
ATOM	1204	CG	TYR	1613	5.841	-8.281	6.549	1.00	22.93
ATOM	1205	CD1	TYR	1613	4.945	-9.245	6.097	1.00	21.60
ATOM	1206	CE1	TYR	1613	3.582	-8.962	5.963	1.00	21.14
ATOM	1207	CD2	TYR	1613	5.347	-7.018	6.869	1.00	25.81
ATOM	1208	CE2	TYR	1613	3.979	-6.718	6.733	1.00	24.45
ATOM	1209	CZ	TYR	1613	3.112	-7.697	6.281	1.00	23.28
ATOM	1210	OH	TYR	1613	1.775	-7.411	6.126	1.00	22.95
ATOM	1212	C	TYR	1613	7.803	-7.138	4.637	1.00	22.57
ATOM	1213	O	TYR	1613	7.022	-7.024	3.699	1.00	24.72
ATOM	1214	N	LEU	1614	8.460	-6.101	5.156	1.00	22.16
ATOM	1216	CA	LEU	1614	8.334	-4.755	4.615	1.00	22.60
ATOM	1217	CB	LEU	1614	9.175	-3.772	5.440	1.00	22.56
ATOM	1218	CG	LEU	1614	8.577	-3.415	6.802	1.00	24.92
ATOM	1219	CD1	LEU	1614	9.535	-2.541	7.580	1.00	21.46
ATOM	1220	CD2	LEU	1614	7.218	-2.711	6.611	1.00	21.87
ATOM	1221	C	LEU	1614	8.699	-4.683	3.124	1.00	23.76
ATOM	1222	O	LEU	1614	7.975	-4.077	2.326	1.00	23.84
ATOM	1223	N	ALA	1615	9.809	-5.314	2.744	1.00	23.48
ATOM	1225	CA	ALA	1615	10.232	-5.340	1.352	1.00	22.70
ATOM	1226	CB	ALA	1615	11.591	-6.019	1.215	1.00	21.52
ATOM	1227	C	ALA	1615	9.188	-6.063	0.505	1.00	22.87
ATOM	1228	O	ALA	1615	8.854	-5.591	-0.581	1.00	24.23
ATOM	1229	N	SER	1616	8.652	-7.176	1.015	1.00	22.76
ATOM	1231	CA	SER	1616	7.638	-7.954	0.295	1.00	22.88
ATOM	1232	CB	SER	1616	7.315	-9.251	1.039	1.00	21.39
ATOM	1233	OG	SER	1616	6.400	-9.036	2.102	1.00	26.24
ATOM	1235	C	SER	1616	6.360	-7.131	0.044	1.00	24.88
ATOM	1236	O	SER	1616	5.635	-7.358	-0.927	1.00	24.73
ATOM	1237	N	LYS	1617	6.104	-6.173	0.927	1.00	23.82
ATOM	1239	CA	LYS	1617	4.970	-5.287	0.810	1.00	22.47
ATOM	1240	CB	LYS	1617	4.455	-4.914	2.199	1.00	23.62
ATOM	1241	CG	LYS	1617	3.792	-6.072	2.927	1.00	27.16
ATOM	1242	CD	LYS	1617	2.551	-6.487	2.169	1.00	30.84
ATOM	1243	CE	LYS	1617	1.810	-7.602	2.852	1.00	33.57
ATOM	1244	NZ	LYS	1617	2.484	-8.894	2.653	1.00	44.30
ATOM	1248	C	LYS	1617	5.346	-4.034	0.035	1.00	23.56
ATOM	1249	O	LYS	1617	4.639	-3.030	0.091	1.00	25.16
ATOM	1250	N	LYS	1618	6.495	-4.066	-0.638	1.00	24.69
ATOM	1252	CA	LYS	1618	6.953	-2.943	-1.468	1.00	24.04

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ATOM	1253	CB	LYS	1618	5.863	-2.581	-2.492	1.00	26.96
ATOM	1254	CG	LYS	1618	5.775	-3.491	-3.709	1.00	29.14
ATOM	1255	CD	LYS	1618	5.567	-4.942	-3.345	1.00	33.91
ATOM	1256	CE	LYS	1618	5.662	-5.858	-4.558	1.00	32.98
ATOM	1257	NZ	LYS	1618	4.431	-5.821	-5.380	1.00	36.73
ATOM	1261	C	LYS	1618	7.406	-1.686	-0.713	1.00	24.01
ATOM	1262	O	LYS	1618	7.557	-0.606	-1.302	1.00	23.73
ATOM	1263	N	CYS	1619	7.689	-1.842	0.573	1.00	25.91
ATOM	1265	CA	CYS	1619	8.108	-0.731	1.418	1.00	25.65
ATOM	1266	CB	CYS	1619	7.444	-0.885	2.792	1.00	24.93
ATOM	1267	SG	CYS	1619	7.941	0.313	4.064	1.00	28.14
ATOM	1268	C	CYS	1619	9.631	-0.628	1.573	1.00	23.07
ATOM	1269	O	CYS	1619	10.304	-1.630	1.809	1.00	20.98
ATOM	1270	N	ILE	1620	10.170	0.573	1.363	1.00	22.95
ATOM	1272	CA	ILE	1620	11.604	0.841	1.524	1.00	23.81
ATOM	1273	CB	ILE	1620	12.202	1.607	0.276	1.00	24.36
ATOM	1274	CG2	ILE	1620	13.670	1.995	0.506	1.00	17.24
ATOM	1275	CG1	ILE	1620	12.108	0.739	-0.987	1.00	23.13
ATOM	1276	CD1	ILE	1620	12.171	1.544	-2.286	1.00	25.37
ATOM	1277	C	ILE	1620	11.633	1.729	2.771	1.00	24.70
ATOM	1278	O	ILE	1620	10.981	2.763	2.806	1.00	25.21
ATOM	1279	N	HIS	1621	12.348	1.297	3.804	1.00	25.62
ATOM	1281	CA	HIS	1621	12.427	2.041	5.057	1.00	25.53
ATOM	1282	CB	HIS	1621	13.181	1.237	6.132	1.00	22.76
ATOM	1283	CG	HIS	1621	13.004	1.773	7.528	1.00	26.42
ATOM	1284	CD2	HIS	1621	12.356	1.260	8.601	1.00	24.74
ATOM	1285	ND1	HIS	1621	13.474	3.011	7.927	1.00	26.62
ATOM	1287	CE1	HIS	1621	13.119	3.233	9.179	1.00	25.70
ATOM	1288	NE2	HIS	1621	12.439	2.187	9.616	1.00	26.23
ATOM	1290	C	HIS	1621	13.073	3.401	4.914	1.00	26.36
ATOM	1291	O	HIS	1621	12.528	4.405	5.370	1.00	25.89
ATOM	1292	N	ARG	1622	14.271	3.406	4.341	1.00	25.35
ATOM	1294	CA	ARG	1622	15.082	4.608	4.140	1.00	25.05
ATOM	1295	CB	ARG	1622	14.268	5.766	3.540	1.00	20.89
ATOM	1296	CG	ARG	1622	13.709	5.444	2.175	1.00	19.03
ATOM	1297	CD	ARG	1622	13.089	6.656	1.488	0.50	14.06
ATOM	1298	NE	ARG	1622	12.684	6.300	0.131	0.50	11.96
ATOM	1300	CZ	ARG	1622	11.606	5.577	-0.166	0.50	11.83
ATOM	1301	NH1	ARG	1622	10.801	5.137	0.797	0.50	10.20
ATOM	1304	NH2	ARG	1622	11.366	5.239	-1.425	0.50	8.63
ATOM	1307	C	ARG	1622	15.877	5.058	5.379	1.00	24.37
ATOM	1308	O	ARG	1622	16.787	5.863	5.268	1.00	25.17
ATOM	1309	N	ASP	1623	15.555	4.527	6.552	1.00	24.61
ATOM	1311	CA	ASP	1623	16.315	4.899	7.748	1.00	28.82
ATOM	1312	CB	ASP	1623	15.777	6.173	8.410	1.00	32.33
ATOM	1313	CG	ASP	1623	16.733	6.735	9.469	1.00	36.67
ATOM	1314	OD1	ASP	1623	16.276	7.520	10.321	1.00	43.56
ATOM	1315	OD2	ASP	1623	17.937	6.385	9.463	1.00	36.29
ATOM	1316	C	ASP	1623	16.408	3.766	8.766	1.00	28.22
ATOM	1317	O	ASP	1623	16.118	3.937	9.956	1.00	26.87
ATOM	1318	N	LEU	1624	16.783	2.592	8.278	1.00	26.34
ATOM	1320	CA	LEU	1624	16.941	1.428	9.132	1.00	26.59
ATOM	1321	CB	LEU	1624	16.996	0.168	8.265	1.00	24.59
ATOM	1322	CG	LEU	1624	17.082	-1.175	8.978	1.00	24.72

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ATOM	1323	CD1	LEU	1624	15.844	-1.408	9.856	1.00	24.35
ATOM	1324	CD2	LEU	1624	17.258	-2.261	7.931	1.00	24.63
ATOM	1325	C	LEU	1624	18.210	1.595	10.004	1.00	26.87
ATOM	1326	O	LEU	1624	19.322	1.777	9.497	1.00	28.19
ATOM	1327	N	ALA	1625	18.009	1.570	11.317	1.00	27.77
ATOM	1329	CA	ALA	1625	19.069	1.741	12.309	1.00	24.54
ATOM	1330	CB	ALA	1625	19.355	3.210	12.494	1.00	19.81
ATOM	1331	C	ALA	1625	18.498	1.173	13.592	1.00	26.44
ATOM	1332	O	ALA	1625	17.289	0.961	13.679	1.00	27.58
ATOM	1333	N	ALA	1626	19.342	0.940	14.594	1.00	25.38
ATOM	1335	CA	ALA	1626	18.872	0.397	15.865	1.00	24.65
ATOM	1336	CB	ALA	1626	20.054	0.023	16.774	1.00	23.35
ATOM	1337	C	ALA	1626	17.929	1.373	16.578	1.00	25.54
ATOM	1338	O	ALA	1626	17.057	0.951	17.325	1.00	27.70
ATOM	1339	N	ARG	1627	18.104	2.671	16.344	1.00	25.06
ATOM	1341	CA	ARG	1627	17.242	3.675	16.959	1.00	25.48
ATOM	1342	CB	ARG	1627	17.706	5.089	16.597	1.00	28.15
ATOM	1343	CG	ARG	1627	17.759	5.370	15.084	1.00	33.13
ATOM	1344	CD	ARG	1627	18.157	6.811	14.774	1.00	33.29
ATOM	1345	NE	ARG	1627	18.442	7.011	13.351	1.00	35.74
ATOM	1347	CZ	ARG	1627	19.652	6.889	12.813	1.00	37.40
ATOM	1348	NH1	ARG	1627	20.695	6.585	13.575	1.00	39.73
ATOM	1351	NH2	ARG	1627	19.817	7.012	11.507	1.00	36.90
ATOM	1354	C	ARG	1627	15.812	3.491	16.479	1.00	24.81
ATOM	1355	O	ARG	1627	14.871	3.853	17.173	1.00	24.05
ATOM	1356	N	ASN	1628	15.667	2.910	15.293	1.00	24.80
ATOM	1358	CA	ASN	1628	14.368	2.686	14.685	1.00	25.97
ATOM	1359	CB	ASN	1628	14.383	3.132	13.225	1.00	30.08
ATOM	1360	CG	ASN	1628	14.417	4.640	13.096	1.00	33.62
ATOM	1361	OD1	ASN	1628	13.775	5.347	13.864	1.00	35.11
ATOM	1362	ND2	ASN	1628	15.212	5.141	12.169	1.00	36.31
ATOM	1365	C	ASN	1628	13.802	1.288	14.824	1.00	26.03
ATOM	1366	O	ASN	1628	12.951	0.869	14.031	1.00	26.87
ATOM	1367	N	VAL	1629	14.330	0.550	15.797	1.00	26.04
ATOM	1369	CA	VAL	1629	13.854	-0.783	16.128	1.00	25.09
ATOM	1370	CB	VAL	1629	14.924	-1.876	15.959	1.00	27.00
ATOM	1371	CG1	VAL	1629	14.390	-3.197	16.546	1.00	20.99
ATOM	1372	CG2	VAL	1629	15.295	-2.051	14.462	1.00	23.26
ATOM	1373	C	VAL	1629	13.504	-0.671	17.600	1.00	27.59
ATOM	1374	O	VAL	1629	14.340	-0.285	18.418	1.00	25.81
ATOM	1375	N	LEU	1630	12.245	-0.929	17.923	1.00	28.17
ATOM	1377	CA	LEU	1630	11.768	-0.845	19.296	1.00	30.20
ATOM	1378	CB	LEU	1630	10.445	-0.077	19.332	1.00	30.26
ATOM	1379	CG	LEU	1630	10.484	1.285	18.626	1.00	29.81
ATOM	1380	CD1	LEU	1630	9.119	1.983	18.745	1.00	28.46
ATOM	1381	CD2	LEU	1630	11.576	2.141	19.233	1.00	28.37
ATOM	1382	C	LEU	1630	11.639	-2.242	19.904	1.00	29.32
ATOM	1383	O	LEU	1630	11.414	-3.219	19.189	1.00	30.84
ATOM	1384	N	VAL	1631	11.800	-2.342	21.221	1.00	28.90
ATOM	1386	CA	VAL	1631	11.732	-3.629	21.905	1.00	26.84
ATOM	1387	CB	VAL	1631	13.067	-3.919	22.670	1.00	28.88
ATOM	1388	CG1	VAL	1631	13.077	-5.341	23.236	1.00	21.54
ATOM	1389	CG2	VAL	1631	14.259	-3.699	21.744	1.00	24.30
ATOM	1390	C	VAL	1631	10.561	-3.645	22.881	1.00	29.02

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ATOM	1391	O	VAL	1631	10.406	-2.737	23.706	1.00	29.31
ATOM	1392	N	THR	1632	9.733	-4.674	22.764	1.00	30.84
ATOM	1394	CA	THR	1632	8.562	-4.830	23.616	1.00	32.24
ATOM	1395	CB	THR	1632	7.488	-5.685	22.912	1.00	31.45
ATOM	1396	OG1	THR	1632	7.896	-7.064	22.910	1.00	30.86
ATOM	1398	CG2	THR	1632	7.268	-5.194	21.470	1.00	28.04
ATOM	1399	C	THR	1632	8.919	-5.493	24.943	1.00	34.17
ATOM	1400	O	THR	1632	10.017	-6.019	25.105	1.00	35.02
ATOM	1401	N	GLU	1633	7.959	-5.524	25.866	1.00	36.16
ATOM	1403	CA	GLU	1633	8.155	-6.138	27.177	1.00	36.34
ATOM	1404	CB	GLU	1633	6.865	-6.063	27.996	1.00	37.07
ATOM	1405	CG	GLU	1633	6.957	-6.649	29.414	1.00	44.57
ATOM	1406	CD	GLU	1633	8.035	-6.000	30.301	1.00	49.38
ATOM	1407	OE1	GLU	1633	8.124	-4.753	30.352	1.00	51.03
ATOM	1408	OE2	GLU	1633	8.788	-6.750	30.968	1.00	51.63
ATOM	1409	C	GLU	1633	8.600	-7.585	27.042	1.00	36.42
ATOM	1410	O	GLU	1633	9.347	-8.085	27.874	1.00	38.56
ATOM	1411	N	ASP	1634	8.185	-8.240	25.964	1.00	37.70
ATOM	1413	CA	ASP	1634	8.550	-9.637	25.737	1.00	38.53
ATOM	1414	CB	ASP	1634	7.408	-10.378	25.027	1.00	44.08
ATOM	1415	CG	ASP	1634	6.041	-10.106	25.657	1.00	51.60
ATOM	1416	OD1	ASP	1634	5.865	-10.367	26.867	1.00	52.37
ATOM	1417	OD2	ASP	1634	5.137	-9.631	24.933	1.00	57.23
ATOM	1418	C	ASP	1634	9.826	-9.776	24.905	1.00	36.56
ATOM	1419	O	ASP	1634	10.127	-10.865	24.430	1.00	36.74
ATOM	1420	N	ASN	1635	10.569	-8.683	24.739	1.00	36.56
ATOM	1422	CA	ASN	1635	11.819	-8.662	23.945	1.00	37.10
ATOM	1423	CB	ASN	1635	12.888	-9.587	24.548	1.00	36.92
ATOM	1424	CG	ASN	1635	13.226	-9.226	25.978	1.00	36.54
ATOM	1425	OD1	ASN	1635	13.275	-8.058	26.340	1.00	38.84
ATOM	1426	ND2	ASN	1635	13.423	-10.235	26.806	1.00	39.58
ATOM	1429	C	ASN	1635	11.632	-8.980	22.451	1.00	34.78
ATOM	1430	O	ASN	1635	12.446	-9.677	21.834	1.00	34.00
ATOM	1431	N	VAL	1636	10.533	-8.498	21.880	1.00	31.35
ATOM	1433	CA	VAL	1636	10.279	-8.711	20.469	1.00	29.76
ATOM	1434	CB	VAL	1636	8.778	-8.946	20.181	1.00	30.60
ATOM	1435	CG1	VAL	1636	8.538	-9.081	18.675	1.00	30.38
ATOM	1436	CG2	VAL	1636	8.315	-10.209	20.897	1.00	28.51
ATOM	1437	C	VAL	1636	10.768	-7.449	19.781	1.00	28.02
ATOM	1438	O	VAL	1636	10.506	-6.351	20.254	1.00	25.87
ATOM	1439	N	MET	1637	11.575	-7.624	18.738	1.00	28.15
ATOM	1441	CA	MET	1637	12.119	-6.508	17.980	1.00	26.01
ATOM	1442	CB	MET	1637	13.366	-6.953	17.204	1.00	27.82
ATOM	1443	CG	MET	1637	14.479	-7.554	18.051	1.00	29.73
ATOM	1444	SD	MET	1637	15.124	-6.410	19.288	1.00	29.96
ATOM	1445	CE	MET	1637	15.120	-7.459	20.689	1.00	27.19
ATOM	1446	C	MET	1637	11.040	-6.087	16.993	1.00	24.77
ATOM	1447	O	MET	1637	10.480	-6.929	16.303	1.00	24.50
ATOM	1448	N	LYS	1638	10.755	-4.791	16.931	1.00	25.74
ATOM	1450	CA	LYS	1638	9.746	-4.258	16.029	1.00	23.67
ATOM	1451	CB	LYS	1638	8.486	-3.888	16.799	1.00	21.78
ATOM	1452	CG	LYS	1638	7.715	-5.092	17.298	1.00	24.60
ATOM	1453	CD	LYS	1638	6.406	-4.683	18.005	1.00	23.87
ATOM	1454	CE	LYS	1638	5.486	-5.897	18.256	1.00	23.06

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ATOM	1455	NZ	LYS	1638	4.871	-6.398	16.976	1.00	24.60
ATOM	1459	C	LYS	1638	10.260	-3.042	15.293	1.00	24.37
ATOM	1460	O	LYS	1638	10.658	-2.055	15.901	1.00	26.58
ATOM	1461	N	ILE	1639	10.271	-3.119	13.971	1.00	25.69
ATOM	1463	CA	ILE	1639	10.721	-2.005	13.148	1.00	25.94
ATOM	1464	CB	ILE	1639	10.935	-2.447	11.668	1.00	26.49
ATOM	1465	CG2	ILE	1639	11.218	-1.236	10.762	1.00	21.19
ATOM	1466	CG1	ILE	1639	12.103	-3.433	11.604	1.00	27.58
ATOM	1467	CD1	ILE	1639	12.120	-4.232	10.355	1.00	32.96
ATOM	1468	C	ILE	1639	9.675	-0.892	13.242	1.00	27.32
ATOM	1469	O	ILE	1639	8.466	-1.133	13.103	1.00	25.45
ATOM	1470	N	ALA	1640	10.156	0.320	13.498	1.00	27.43
ATOM	1472	CA	ALA	1640	9.321	1.499	13.632	1.00	26.96
ATOM	1473	CB	ALA	1640	9.557	2.133	15.006	1.00	25.21
ATOM	1474	C	ALA	1640	9.641	2.510	12.538	1.00	26.80
ATOM	1475	O	ALA	1640	10.691	2.446	11.896	1.00	27.55
ATOM	1476	N	ASP	1641	8.716	3.440	12.328	1.00	27.06
ATOM	1478	CA	ASP	1641	8.862	4.526	11.349	1.00	30.54
ATOM	1479	CB	ASP	1641	9.993	5.484	11.753	1.00	33.12
ATOM	1480	CG	ASP	1641	9.668	6.310	12.999	1.00	36.17
ATOM	1481	OD1	ASP	1641	10.477	7.203	13.334	1.00	42.24
ATOM	1482	OD2	ASP	1641	8.633	6.076	13.648	1.00	33.22
ATOM	1483	C	ASP	1641	9.049	4.107	9.898	1.00	29.94
ATOM	1484	O	ASP	1641	9.598	4.861	9.102	1.00	30.13
ATOM	1485	N	PHE	1642	8.569	2.920	9.553	1.00	30.22
ATOM	1487	CA	PHE	1642	8.680	2.426	8.191	1.00	30.91
ATOM	1488	CB	PHE	1642	8.462	0.909	8.159	1.00	26.24
ATOM	1489	CG	PHE	1642	7.156	0.470	8.750	1.00	27.82
ATOM	1490	CD1	PHE	1642	5.986	0.495	7.988	1.00	27.08
ATOM	1491	CD2	PHE	1642	7.089	0.026	10.066	1.00	26.70
ATOM	1492	CE1	PHE	1642	4.761	0.088	8.532	1.00	25.18
ATOM	1493	CE2	PHE	1642	5.872	-0.383	10.624	1.00	27.59
ATOM	1494	CZ	PHE	1642	4.705	-0.354	9.855	1.00	28.05
ATOM	1495	C	PHE	1642	7.729	3.139	7.219	1.00	33.35
ATOM	1496	O	PHE	1642	7.983	3.165	6.018	1.00	36.19
ATOM	1497	N	GLY	1643	6.661	3.746	7.736	1.00	32.76
ATOM	1499	CA	GLY	1643	5.710	4.419	6.863	1.00	31.44
ATOM	1500	C	GLY	1643	5.805	5.927	6.910	1.00	32.94
ATOM	1501	O	GLY	1643	4.945	6.636	6.399	1.00	33.10
ATOM	1502	N	LEU	1644	6.872	6.407	7.525	1.00	35.45
ATOM	1504	CA	LEU	1644	7.124	7.828	7.684	1.00	39.04
ATOM	1505	CB	LEU	1644	8.387	8.011	8.514	1.00	37.80
ATOM	1506	CG	LEU	1644	8.414	9.120	9.549	1.00	42.51
ATOM	1507	CD1	LEU	1644	7.301	8.887	10.563	1.00	44.08
ATOM	1508	CD2	LEU	1644	9.779	9.127	10.243	1.00	44.47
ATOM	1509	C	LEU	1644	7.259	8.580	6.357	1.00	42.20
ATOM	1510	O	LEU	1644	7.895	8.107	5.414	1.00	44.14
ATOM	1511	N	ALA	1645	6.607	9.732	6.267	1.00	43.89
ATOM	1513	CA	ALA	1645	6.677	10.569	5.082	1.00	45.62
ATOM	1514	CB	ALA	1645	5.463	11.493	5.028	1.00	45.06
ATOM	1515	C	ALA	1645	7.966	11.388	5.186	1.00	45.82
ATOM	1516	O	ALA	1645	8.240	11.994	6.228	1.00	45.85
ATOM	1517	N	ARG	1646	8.766	11.389	4.129	1.00	45.16
ATOM	1519	CA	ARG	1646	10.015	12.140	4.138	1.00	47.06

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ATOM	1520	CB	ARG	1646	11.126	11.318	4.794	1.00	48.00
ATOM	1521	C	ARG	1646	10.445	12.546	2.742	1.00	46.83
ATOM	1522	O	ARG	1646	10.429	11.729	1.823	1.00	45.76
ATOM	1523	N	ASP	1647	10.807	13.814	2.578	1.00	48.96
ATOM	1525	CA	ASP	1647	11.278	14.291	1.288	1.00	50.93
ATOM	1526	CB	ASP	1647	10.938	15.769	1.073	1.00	52.33
ATOM	1527	CG	ASP	1647	11.191	16.228	-0.360	1.00	55.93
ATOM	1528	OD1	ASP	1647	12.231	15.850	-0.956	1.00	52.58
ATOM	1529	OD2	ASP	1647	10.340	16.980	-0.896	1.00	59.54
ATOM	1530	C	ASP	1647	12.789	14.104	1.336	1.00	50.78
ATOM	1531	O	ASP	1647	13.491	14.803	2.077	1.00	48.32
ATOM	1532	N	ILE	1648	13.274	13.144	0.556	1.00	50.84
ATOM	1534	CA	ILE	1648	14.696	12.833	0.516	1.00	52.58
ATOM	1535	CB	ILE	1648	14.984	11.571	-0.324	1.00	50.85
ATOM	1536	CG2	ILE	1648	14.204	10.386	0.241	1.00	49.34
ATOM	1537	CG1	ILE	1648	14.638	11.813	-1.801	1.00	48.22
ATOM	1538	CD1	ILE	1648	15.233	10.806	-2.754	1.00	42.86
ATOM	1539	C	ILE	1648	15.523	13.999	-0.018	1.00	55.57
ATOM	1540	O	ILE	1648	16.648	14.222	0.423	1.00	57.24
ATOM	1541	N	HIS	1649	14.944	14.766	-0.936	1.00	56.80
ATOM	1543	CA	HIS	1649	15.650	15.895	-1.520	1.00	58.03
ATOM	1544	CB	HIS	1649	15.013	16.302	-2.859	1.00	58.71
ATOM	1545	CG	HIS	1649	15.221	15.308	-3.958	1.00	60.28
ATOM	1546	CD2	HIS	1649	16.303	14.566	-4.306	1.00	60.74
ATOM	1547	ND1	HIS	1649	14.241	14.986	-4.874	1.00	61.70
ATOM	1549	CE1	HIS	1649	14.708	14.104	-5.742	1.00	61.86
ATOM	1550	NE2	HIS	1649	15.959	13.833	-5.417	1.00	60.98
ATOM	1552	C	HIS	1649	15.721	17.093	-0.591	1.00	58.49
ATOM	1553	O	HIS	1649	16.129	18.175	-1.004	1.00	60.56
ATOM	1554	N	HIS	1650	15.285	16.916	0.654	1.00	59.58
ATOM	1556	CA	HIS	1650	15.306	18.001	1.635	1.00	61.38
ATOM	1557	CB	HIS	1650	13.898	18.540	1.863	1.00	65.28
ATOM	1558	CG	HIS	1650	13.404	19.433	0.738	1.00	72.62
ATOM	1559	CD2	HIS	1650	13.492	20.752	0.536	1.00	76.23
ATOM	1560	ND1	HIS	1650	12.710	18.904	-0.339	1.00	77.05
ATOM	1562	CE1	HIS	1650	12.402	19.907	-1.157	1.00	78.51
ATOM	1563	NE2	HIS	1650	12.863	21.015	-0.647	1.00	78.82
ATOM	1565	C	HIS	1650	15.925	17.575	2.972	1.00	60.63
ATOM	1566	O	HIS	1650	15.796	18.271	3.969	1.00	60.20
ATOM	1567	N	ILE	1651	16.584	16.419	2.987	1.00	60.22
ATOM	1569	CA	ILE	1651	17.197	15.920	4.204	1.00	60.03
ATOM	1570	CB	ILE	1651	17.574	14.434	4.069	1.00	62.54
ATOM	1571	CG2	ILE	1651	18.280	13.920	5.323	1.00	63.48
ATOM	1572	CG1	ILE	1651	16.329	13.584	3.800	1.00	65.18
ATOM	1573	CD1	ILE	1651	16.635	12.124	3.603	1.00	67.18
ATOM	1574	C	ILE	1651	18.457	16.698	4.557	1.00	59.16
ATOM	1575	O	ILE	1651	19.326	16.907	3.716	1.00	59.25
ATOM	1576	N	ASP	1652	18.532	17.176	5.793	1.00	58.91
ATOM	1578	CA	ASP	1652	19.702	17.915	6.260	1.00	58.25
ATOM	1579	CB	ASP	1652	19.312	18.788	7.444	1.00	61.14
ATOM	1580	CG	ASP	1652	20.506	19.569	8.028	1.00	65.33
ATOM	1581	OD1	ASP	1652	21.614	19.574	7.411	1.00	67.11
ATOM	1582	OD2	ASP	1652	20.337	20.191	9.126	1.00	69.04
ATOM	1583	C	ASP	1652	20.786	16.922	6.676	1.00	56.75

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ATOM	1584	O	ASP	1652	20.699	16.307	7.741	1.00	56.06
ATOM	1585	N	TYR	1653	21.794	16.762	5.826	1.00	55.40
ATOM	1587	CA	TYR	1653	22.900	15.849	6.088	1.00	54.50
ATOM	1588	CB	TYR	1653	23.825	15.783	4.872	1.00	52.80
ATOM	1589	CG	TYR	1653	23.334	14.854	3.796	1.00	52.10
ATOM	1590	CD1	TYR	1653	24.123	14.566	2.685	1.00	51.50
ATOM	1591	CE1	TYR	1653	23.701	13.658	1.724	1.00	53.52
ATOM	1592	CD2	TYR	1653	22.099	14.214	3.917	1.00	52.88
ATOM	1593	CE2	TYR	1653	21.664	13.302	2.966	1.00	54.63
ATOM	1594	CZ	TYR	1653	22.469	13.025	1.870	1.00	54.35
ATOM	1595	OH	TYR	1653	22.049	12.107	0.933	1.00	53.23
ATOM	1597	C	TYR	1653	23.717	16.158	7.339	1.00	55.40
ATOM	1598	O	TYR	1653	24.381	15.284	7.900	1.00	54.47
ATOM	1599	N	TYR	1654	23.673	17.409	7.773	1.00	56.72
ATOM	1601	CA	TYR	1654	24.421	17.826	8.947	1.00	58.87
ATOM	1602	CB	TYR	1654	24.978	19.235	8.733	1.00	57.91
ATOM	1603	CG	TYR	1654	26.068	19.269	7.685	1.00	60.49
ATOM	1604	CD1	TYR	1654	25.760	19.301	6.325	1.00	61.37
ATOM	1605	CE1	TYR	1654	26.769	19.289	5.356	1.00	63.72
ATOM	1606	CD2	TYR	1654	27.412	19.227	8.053	1.00	61.74
ATOM	1607	CE2	TYR	1654	28.425	19.216	7.099	1.00	64.08
ATOM	1608	CZ	TYR	1654	28.102	19.248	5.753	1.00	65.12
ATOM	1609	OH	TYR	1654	29.117	19.248	4.817	1.00	64.17
ATOM	1611	C	TYR	1654	23.628	17.732	10.245	1.00	60.17
ATOM	1612	O	TYR	1654	24.173	17.935	11.335	1.00	61.09
ATOM	1613	N	LYS	1655	22.348	17.393	10.133	1.00	60.54
ATOM	1615	CA	LYS	1655	21.493	17.277	11.306	1.00	62.12
ATOM	1616	CB	LYS	1655	20.019	17.382	10.910	1.00	64.32
ATOM	1617	CG	LYS	1655	19.054	17.346	12.079	1.00	67.17
ATOM	1618	CD	LYS	1655	17.644	17.608	11.602	1.00	73.05
ATOM	1619	CE	LYS	1655	16.626	17.243	12.660	1.00	77.36
ATOM	1620	NZ	LYS	1655	15.230	17.494	12.186	1.00	81.10
ATOM	1624	C	LYS	1655	21.754	15.976	12.057	1.00	62.19
ATOM	1625	O	LYS	1655	21.902	14.907	11.454	1.00	61.36
ATOM	1626	N	LYS	1656	21.822	16.084	13.380	1.00	62.26
ATOM	1628	CA	LYS	1656	22.069	14.933	14.236	1.00	62.28
ATOM	1629	CB	LYS	1656	23.027	15.310	15.372	1.00	62.05
ATOM	1630	CG	LYS	1656	24.474	15.489	14.957	1.00	62.62
ATOM	1631	CD	LYS	1656	25.320	15.889	16.157	1.00	66.45
ATOM	1632	CE	LYS	1656	26.803	15.666	15.908	1.00	67.28
ATOM	1633	NZ	LYS	1656	27.619	16.007	17.109	1.00	68.45
ATOM	1637	C	LYS	1656	20.774	14.381	14.824	1.00	61.86
ATOM	1638	O	LYS	1656	19.714	15.007	14.733	1.00	62.95
ATOM	1639	N	THR	1657	20.875	13.198	15.420	1.00	60.10
ATOM	1641	CA	THR	1657	19.743	12.541	16.053	1.00	57.73
ATOM	1642	CB	THR	1657	19.973	11.012	16.121	1.00	56.04
ATOM	1643	OG1	THR	1657	21.150	10.730	16.896	1.00	55.21
ATOM	1645	CG2	THR	1657	20.152	10.431	14.731	1.00	53.07
ATOM	1646	C	THR	1657	19.664	13.102	17.472	1.00	57.74
ATOM	1647	O	THR	1657	20.513	13.899	17.870	1.00	57.76
ATOM	1648	N	THR	1658	18.678	12.667	18.249	1.00	58.80
ATOM	1650	CA	THR	1658	18.548	13.140	19.627	1.00	60.33
ATOM	1651	CB	THR	1658	17.318	12.517	20.290	1.00	61.37
ATOM	1652	C	THR	1658	19.811	12.779	20.406	1.00	60.43

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ATOM	1653	O	THR	1658	20.350	13.599	21.155	1.00	60.59
ATOM	1654	N	ASN	1659	20.311	11.567	20.161	1.00	59.97
ATOM	1656	CA	ASN	1659	21.508	11.058	20.827	1.00	58.28
ATOM	1657	CB	ASN	1659	21.607	9.545	20.645	1.00	59.95
ATOM	1658	CG	ASN	1659	22.444	8.883	21.723	1.00	60.10
ATOM	1659	OD1	ASN	1659	22.382	9.265	22.891	1.00	61.26
ATOM	1660	ND2	ASN	1659	23.210	7.867	21.341	1.00	57.09
ATOM	1663	C	ASN	1659	22.781	11.717	20.311	1.00	57.13
ATOM	1664	O	ASN	1659	23.868	11.418	20.793	1.00	57.34
ATOM	1665	N	GLY	1660	22.643	12.570	19.299	1.00	56.48
ATOM	1667	CA	GLY	1660	23.781	13.276	18.733	1.00	54.87
ATOM	1668	C	GLY	1660	24.539	12.570	17.623	1.00	53.04
ATOM	1669	O	GLY	1660	25.716	12.855	17.394	1.00	54.11
ATOM	1670	N	ARG	1661	23.879	11.659	16.918	1.00	51.37
ATOM	1672	CA	ARG	1661	24.536	10.930	15.833	1.00	48.96
ATOM	1673	CB	ARG	1661	24.283	9.428	15.961	1.00	48.48
ATOM	1674	CG	ARG	1661	24.848	8.796	17.215	1.00	50.03
ATOM	1675	CD	ARG	1661	24.492	7.325	17.234	1.00	50.78
ATOM	1676	NE	ARG	1661	25.013	6.614	18.396	1.00	50.11
ATOM	1678	CZ	ARG	1661	24.902	5.299	18.566	1.00	50.08
ATOM	1679	NH1	ARG	1661	24.286	4.560	17.645	1.00	46.57
ATOM	1682	NH2	ARG	1661	25.426	4.717	19.643	1.00	47.88
ATOM	1685	C	ARG	1661	24.076	11.422	14.459	1.00	46.53
ATOM	1686	O	ARG	1661	23.031	12.029	14.325	1.00	45.01
ATOM	1687	N	LEU	1662	24.839	11.094	13.432	1.00	42.39
ATOM	1689	CA	LEU	1662	24.546	11.503	12.076	1.00	40.71
ATOM	1690	CB	LEU	1662	25.823	12.031	11.399	1.00	40.25
ATOM	1691	CG	LEU	1662	26.408	13.332	11.965	1.00	42.44
ATOM	1692	CD1	LEU	1662	27.853	13.478	11.537	1.00	40.42
ATOM	1693	CD2	LEU	1662	25.591	14.536	11.514	1.00	41.16
ATOM	1694	C	LEU	1662	23.946	10.362	11.258	1.00	38.45
ATOM	1695	O	LEU	1662	24.647	9.436	10.862	1.00	36.67
ATOM	1696	N	PRO	1663	22.632	10.428	10.987	1.00	37.09
ATOM	1697	CD	PRO	1663	21.717	11.475	11.489	1.00	38.18
ATOM	1698	CA	PRO	1663	21.894	9.424	10.207	1.00	35.59
ATOM	1699	CB	PRO	1663	20.535	10.098	9.983	1.00	35.90
ATOM	1700	CG	PRO	1663	20.343	10.856	11.258	1.00	39.13
ATOM	1701	C	PRO	1663	22.556	9.045	8.876	1.00	33.05
ATOM	1702	O	PRO	1663	22.362	7.933	8.378	1.00	31.16
ATOM	1703	N	VAL	1664	23.333	9.960	8.299	1.00	32.07
ATOM	1705	CA	VAL	1664	24.020	9.669	7.034	1.00	32.49
ATOM	1706	CB	VAL	1664	24.831	10.886	6.477	1.00	32.68
ATOM	1707	CG1	VAL	1664	23.898	11.906	5.864	1.00	32.25
ATOM	1708	CG2	VAL	1664	25.670	11.523	7.571	1.00	33.22
ATOM	1709	C	VAL	1664	24.957	8.469	7.171	1.00	29.57
ATOM	1710	O	VAL	1664	25.328	7.864	6.175	1.00	27.39
ATOM	1711	N	LYS	1665	25.303	8.116	8.409	1.00	28.82
ATOM	1713	CA	LYS	1665	26.189	6.991	8.673	1.00	27.87
ATOM	1714	CB	LYS	1665	26.815	7.100	10.065	1.00	26.99
ATOM	1715	CG	LYS	1665	27.967	8.089	10.079	1.00	29.23
ATOM	1716	CD	LYS	1665	28.283	8.619	11.466	1.00	30.64
ATOM	1717	CE	LYS	1665	29.543	9.478	11.426	1.00	30.94
ATOM	1718	NZ	LYS	1665	29.826	10.128	12.737	1.00	31.63
ATOM	1722	C	LYS	1665	25.546	5.637	8.465	1.00	26.76

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ATOM	1723	O	LYS	1665	26.211	4.615	8.589	1.00	26.78
ATOM	1724	N	TRP	1666	24.260	5.630	8.137	1.00	25.79
ATOM	1726	CA	TRP	1666	23.561	4.381	7.865	1.00	26.56
ATOM	1727	CB	TRP	1666	22.299	4.273	8.724	1.00	25.63
ATOM	1728	CG	TRP	1666	22.564	3.872	10.174	1.00	26.95
ATOM	1729	CD2	TRP	1666	23.052	4.717	11.232	1.00	24.83
ATOM	1730	CE2	TRP	1666	23.134	3.920	12.398	1.00	24.49
ATOM	1731	CE3	TRP	1666	23.433	6.062	11.306	1.00	24.54
ATOM	1732	CD1	TRP	1666	22.376	2.636	10.730	1.00	20.10
ATOM	1733	NE1	TRP	1666	22.716	2.660	12.063	1.00	21.86
ATOM	1735	CZ2	TRP	1666	23.575	4.433	13.627	1.00	25.71
ATOM	1736	CZ3	TRP	1666	23.870	6.569	12.523	1.00	26.00
ATOM	1737	CH2	TRP	1666	23.939	5.754	13.665	1.00	26.04
ATOM	1738	C	TRP	1666	23.188	4.263	6.386	1.00	23.62
ATOM	1739	O	TRP	1666	22.754	3.214	5.931	1.00	24.87
ATOM	1740	N	MET	1667	23.404	5.330	5.631	1.00	22.78
ATOM	1742	CA	MET	1667	23.046	5.361	4.215	1.00	23.73
ATOM	1743	CB	MET	1667	22.894	6.802	3.744	1.00	26.24
ATOM	1744	CG	MET	1667	21.823	7.621	4.434	1.00	35.55
ATOM	1745	SD	MET	1667	21.795	9.276	3.706	1.00	42.23
ATOM	1746	CE	MET	1667	21.019	8.904	2.238	1.00	40.57
ATOM	1747	C	MET	1667	23.991	4.693	3.239	1.00	22.77
ATOM	1748	O	MET	1667	25.205	4.894	3.294	1.00	24.25
ATOM	1749	N	ALA	1668	23.420	3.963	2.286	1.00	22.73
ATOM	1751	CA	ALA	1668	24.217	3.337	1.237	1.00	23.54
ATOM	1752	CB	ALA	1668	23.339	2.495	0.340	1.00	21.80
ATOM	1753	C	ALA	1668	24.805	4.495	0.430	1.00	25.53
ATOM	1754	O	ALA	1668	24.181	5.551	0.316	1.00	23.66
ATOM	1755	N	PRO	1669	26.006	4.314	-0.153	1.00	26.86
ATOM	1756	CD	PRO	1669	26.899	3.144	-0.095	1.00	26.35
ATOM	1757	CA	PRO	1669	26.611	5.390	-0.942	1.00	27.78
ATOM	1758	CB	PRO	1669	27.864	4.731	-1.518	1.00	25.51
ATOM	1759	CG	PRO	1669	28.225	3.741	-0.471	1.00	25.36
ATOM	1760	C	PRO	1669	25.686	5.900	-2.057	1.00	26.47
ATOM	1761	O	PRO	1669	25.617	7.099	-2.288	1.00	28.42
ATOM	1762	N	GLU	1670	24.951	5.010	-2.724	1.00	26.88
ATOM	1764	CA	GLU	1670	24.057	5.459	-3.796	1.00	29.03
ATOM	1765	CB	GLU	1670	23.597	4.293	-4.693	1.00	31.79
ATOM	1766	CG	GLU	1670	22.588	3.325	-4.065	1.00	32.47
ATOM	1767	CD	GLU	1670	23.212	2.184	-3.255	1.00	32.43
ATOM	1768	OE1	GLU	1670	22.429	1.297	-2.822	1.00	25.01
ATOM	1769	OE2	GLU	1670	24.458	2.157	-3.069	1.00	28.75
ATOM	1770	C	GLU	1670	22.864	6.274	-3.294	1.00	28.37
ATOM	1771	O	GLU	1670	22.358	7.146	-4.001	1.00	25.72
ATOM	1772	N	ALA	1671	22.451	6.028	-2.053	1.00	30.08
ATOM	1774	CA	ALA	1671	21.347	6.779	-1.465	1.00	31.24
ATOM	1775	CB	ALA	1671	20.751	6.031	-0.287	1.00	26.42
ATOM	1776	C	ALA	1671	21.899	8.125	-1.013	1.00	31.36
ATOM	1777	O	ALA	1671	21.298	9.167	-1.249	1.00	33.11
ATOM	1778	N	LEU	1672	23.068	8.096	-0.387	1.00	32.73
ATOM	1780	CA	LEU	1672	23.715	9.304	0.100	1.00	33.96
ATOM	1781	CB	LEU	1672	24.931	8.935	0.940	1.00	33.89
ATOM	1782	CG	LEU	1672	25.783	10.071	1.502	1.00	37.62
ATOM	1783	CD1	LEU	1672	25.010	10.800	2.581	1.00	39.57

ATOM	1784	CD2	LEU	1672	27.054	9.491	2.087	1.00	32.30
ATOM	1785	C	LEU	1672	24.157	10.207	-1.042	1.00	36.83
ATOM	1786	O	LEU	1672	23.769	11.369	-1.102	1.00	37.87
ATOM	1787	N	PHE	1673	24.959	9.669	-1.954	1.00	35.82
ATOM	1789	CA	PHE	1673	25.466	10.449	-3.071	1.00	35.82
ATOM	1790	CB	PHE	1673	26.738	9.802	-3.639	1.00	34.66
ATOM	1791	CG	PHE	1673	27.850	9.642	-2.634	1.00	33.84
ATOM	1792	CD1	PHE	1673	28.503	8.422	-2.494	1.00	32.65
ATOM	1793	CD2	PHE	1673	28.242	10.709	-1.827	1.00	36.98
ATOM	1794	CE1	PHE	1673	29.540	8.257	-1.555	1.00	37.95
ATOM	1795	CE2	PHE	1673	29.279	10.557	-0.881	1.00	39.90
ATOM	1796	CZ	PHE	1673	29.927	9.325	-0.748	1.00	37.09
ATOM	1797	C	PHE	1673	24.483	10.692	-4.210	1.00	36.34
ATOM	1798	O	PHE	1673	24.430	11.788	-4.754	1.00	37.18
ATOM	1799	N	ASP	1674	23.705	9.677	-4.568	1.00	38.22
ATOM	1801	CA	ASP	1674	22.780	9.777	-5.693	1.00	38.51
ATOM	1802	CB	ASP	1674	23.008	8.597	-6.633	1.00	40.34
ATOM	1803	CG	ASP	1674	24.439	8.511	-7.122	1.00	43.87
ATOM	1804	OD1	ASP	1674	25.092	9.571	-7.254	1.00	42.79
ATOM	1805	OD2	ASP	1674	24.906	7.376	-7.369	1.00	47.94
ATOM	1806	C	ASP	1674	21.298	9.853	-5.360	1.00	40.21
ATOM	1807	O	ASP	1674	20.457	9.872	-6.271	1.00	39.07
ATOM	1808	N	ARG	1675	20.975	9.836	-4.072	1.00	39.83
ATOM	1810	CA	ARG	1675	19.589	9.900	-3.631	1.00	42.25
ATOM	1811	CB	ARG	1675	18.992	11.271	-3.964	1.00	48.19
ATOM	1812	CG	ARG	1675	19.691	12.420	-3.267	1.00	59.20
ATOM	1813	CD	ARG	1675	19.462	13.729	-4.019	1.00	67.81
ATOM	1814	NE	ARG	1675	20.079	14.876	-3.352	1.00	75.11
ATOM	1816	CZ	ARG	1675	19.688	16.136	-3.525	1.00	78.74
ATOM	1817	NH1	ARG	1675	18.680	16.429	-4.341	1.00	79.91
ATOM	1820	NH2	ARG	1675	20.311	17.115	-2.890	1.00	81.24
ATOM	1823	C	ARG	1675	18.730	8.777	-4.221	1.00	39.00
ATOM	1824	O	ARG	1675	17.544	8.956	-4.488	1.00	39.71
ATOM	1825	N	ILE	1676	19.345	7.624	-4.434	1.00	35.50
ATOM	1827	CA	ILE	1676	18.636	6.471	-4.958	1.00	33.51
ATOM	1828	CB	ILE	1676	19.434	5.759	-6.039	1.00	34.59
ATOM	1829	CG2	ILE	1676	18.582	4.678	-6.649	1.00	33.90
ATOM	1830	CG1	ILE	1676	19.848	6.752	-7.120	1.00	37.60
ATOM	1831	CD1	ILE	1676	20.861	6.197	-8.109	1.00	42.67
ATOM	1832	C	ILE	1676	18.390	5.501	-3.809	1.00	30.94
ATOM	1833	O	ILE	1676	19.326	4.926	-3.252	1.00	28.62
ATOM	1834	N	TYR	1677	17.124	5.351	-3.443	1.00	30.60
ATOM	1836	CA	TYR	1677	16.724	4.467	-2.359	1.00	25.87
ATOM	1837	CB	TYR	1677	15.781	5.197	-1.413	1.00	26.40
ATOM	1838	CG	TYR	1677	16.483	6.220	-0.555	1.00	27.67
ATOM	1839	CD1	TYR	1677	16.663	7.533	-0.999	1.00	27.45
ATOM	1840	CE1	TYR	1677	17.269	8.483	-0.191	1.00	26.55
ATOM	1841	CD2	TYR	1677	16.935	5.883	0.721	1.00	24.58
ATOM	1842	CE2	TYR	1677	17.536	6.828	1.538	1.00	26.35
ATOM	1843	CZ	TYR	1677	17.698	8.122	1.080	1.00	28.80
ATOM	1844	OH	TYR	1677	18.270	9.059	1.914	1.00	34.97
ATOM	1846	C	TYR	1677	16.055	3.235	-2.911	1.00	22.70
ATOM	1847	O	TYR	1677	15.144	3.335	-3.728	1.00	26.22
ATOM	1848	N	THR	1678	16.477	2.076	-2.420	1.00	21.83

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ATOM	1850	CA	THR	1678	15.968	0.791	-2.865	1.00	22.14
ATOM	1851	CB	THR	1678	16.907	0.191	-3.928	1.00	23.91
ATOM	1852	OG1	THR	1678	18.229	0.105	-3.373	1.00	27.47
ATOM	1854	CG2	THR	1678	16.949	1.053	-5.188	1.00	24.94
ATOM	1855	C	THR	1678	15.999	-0.176	-1.692	1.00	22.79
ATOM	1856	O	THR	1678	16.427	0.170	-0.592	1.00	23.39
ATOM	1857	N	HIS	1679	15.563	-1.402	-1.929	1.00	21.98
ATOM	1859	CA	HIS	1679	15.613	-2.417	-0.888	1.00	22.97
ATOM	1860	CB	HIS	1679	14.872	-3.671	-1.351	1.00	22.04
ATOM	1861	CG	HIS	1679	13.421	-3.444	-1.621	1.00	25.41
ATOM	1862	CD2	HIS	1679	12.674	-3.611	-2.740	1.00	26.60
ATOM	1863	ND1	HIS	1679	12.556	-2.954	-0.663	1.00	26.13
ATOM	1865	CE1	HIS	1679	11.348	-2.830	-1.178	1.00	28.66
ATOM	1866	NE2	HIS	1679	11.394	-3.221	-2.441	1.00	29.66
ATOM	1868	C	HIS	1679	17.097	-2.719	-0.650	1.00	23.14
ATOM	1869	O	HIS	1679	17.511	-3.074	0.459	1.00	21.69
ATOM	1870	N	GLN	1680	17.895	-2.506	-1.697	1.00	22.38
ATOM	1872	CA	GLN	1680	19.335	-2.726	-1.658	1.00	22.33
ATOM	1873	CB	GLN	1680	19.948	-2.594	-3.058	1.00	22.52
ATOM	1874	CG	GLN	1680	19.895	-3.872	-3.879	1.00	29.15
ATOM	1875	CD	GLN	1680	18.865	-3.847	-4.991	1.00	33.60
ATOM	1876	OE1	GLN	1680	17.819	-3.212	-4.871	1.00	38.43
ATOM	1877	NE2	GLN	1680	19.159	-4.542	-6.085	1.00	33.44
ATOM	1880	C	GLN	1680	20.007	-1.740	-0.732	1.00	22.61
ATOM	1881	O	GLN	1680	20.943	-2.093	-0.027	1.00	22.00
ATOM	1882	N	SER	1681	19.562	-0.490	-0.745	1.00	22.06
ATOM	1884	CA	SER	1681	20.184	0.479	0.137	1.00	23.41
ATOM	1885	CB	SER	1681	19.886	1.923	-0.306	1.00	20.06
ATOM	1886	OG	SER	1681	18.503	2.166	-0.479	1.00	22.90
ATOM	1888	C	SER	1681	19.778	0.206	1.583	1.00	23.08
ATOM	1889	O	SER	1681	20.528	0.531	2.506	1.00	24.13
ATOM	1890	N	ASP	1682	18.608	-0.412	1.770	1.00	23.19
ATOM	1892	CA	ASP	1682	18.107	-0.775	3.104	1.00	22.37
ATOM	1893	CB	ASP	1682	16.660	-1.275	3.018	1.00	24.55
ATOM	1894	CG	ASP	1682	15.616	-0.172	3.222	1.00	24.22
ATOM	1895	OD1	ASP	1682	14.428	-0.479	3.005	1.00	25.02
ATOM	1896	OD2	ASP	1682	15.949	0.968	3.625	1.00	24.82
ATOM	1897	C	ASP	1682	18.980	-1.888	3.690	1.00	20.47
ATOM	1898	O	ASP	1682	19.172	-1.984	4.906	1.00	21.83
ATOM	1899	N	VAL	1683	19.480	-2.746	2.806	1.00	20.14
ATOM	1901	CA	VAL	1683	20.340	-3.856	3.179	1.00	20.49
ATOM	1902	CB	VAL	1683	20.493	-4.842	2.003	1.00	22.38
ATOM	1903	CG1	VAL	1683	21.757	-5.691	2.159	1.00	19.57
ATOM	1904	CG2	VAL	1683	19.264	-5.740	1.942	1.00	22.35
ATOM	1905	C	VAL	1683	21.677	-3.315	3.683	1.00	20.22
ATOM	1906	O	VAL	1683	22.202	-3.789	4.684	1.00	21.41
ATOM	1907	N	TRP	1684	22.210	-2.311	3.003	1.00	21.33
ATOM	1909	CA	TRP	1684	23.440	-1.666	3.449	1.00	22.21
ATOM	1910	CB	TRP	1684	23.768	-0.473	2.540	1.00	18.78
ATOM	1911	CG	TRP	1684	24.924	0.391	3.037	1.00	22.80
ATOM	1912	CD2	TRP	1684	26.237	0.477	2.472	1.00	24.60
ATOM	1913	CE2	TRP	1684	26.989	1.364	3.286	1.00	24.34
ATOM	1914	CE3	TRP	1684	26.853	-0.099	1.352	1.00	24.32
ATOM	1915	CD1	TRP	1684	24.933	1.208	4.138	1.00	22.28

ATOM	1916	NE1	TRP	1684	26.169	1.791	4.297	1.00	22.32
ATOM	1918	CZ2	TRP	1684	28.324	1.669	3.022	1.00	24.77
ATOM	1919	CZ3	TRP	1684	28.193	0.213	1.090	1.00	24.46
ATOM	1920	CH2	TRP	1684	28.906	1.088	1.918	1.00	24.00
ATOM	1921	C	TRP	1684	23.198	-1.183	4.899	1.00	23.26
ATOM	1922	O	TRP	1684	23.982	-1.475	5.805	1.00	24.52
ATOM	1923	N	SER	1685	22.108	-0.447	5.113	1.00	22.88
ATOM	1925	CA	SER	1685	21.744	0.057	6.444	1.00	24.01
ATOM	1926	CB	SER	1685	20.398	0.783	6.385	1.00	21.90
ATOM	1927	OG	SER	1685	20.424	1.787	5.388	1.00	24.75
ATOM	1929	C	SER	1685	21.659	-1.087	7.464	1.00	24.28
ATOM	1930	O	SER	1685	22.077	-0.933	8.625	1.00	23.94
ATOM	1931	N	PHE	1686	21.099	-2.221	7.037	1.00	23.20
ATOM	1933	CA	PHE	1686	20.993	-3.393	7.898	1.00	23.87
ATOM	1934	CB	PHE	1686	20.216	-4.519	7.216	1.00	19.56
ATOM	1935	CG	PHE	1686	20.062	-5.734	8.075	1.00	22.19
ATOM	1936	CD1	PHE	1686	19.240	-5.701	9.203	1.00	21.55
ATOM	1937	CD2	PHE	1686	20.773	-6.899	7.793	1.00	21.94
ATOM	1938	CE1	PHE	1686	19.125	-6.801	10.033	1.00	21.66
ATOM	1939	CE2	PHE	1686	20.663	-8.012	8.623	1.00	22.47
ATOM	1940	CZ	PHE	1686	19.842	-7.961	9.743	1.00	23.14
ATOM	1941	C	PHE	1686	22.389	-3.890	8.300	1.00	22.62
ATOM	1942	O	PHE	1686	22.579	-4.424	9.407	1.00	23.09
ATOM	1943	N	GLY	1687	23.354	-3.726	7.401	1.00	23.50
ATOM	1945	CA	GLY	1687	24.718	-4.110	7.721	1.00	23.83
ATOM	1946	C	GLY	1687	25.230	-3.247	8.867	1.00	21.95
ATOM	1947	O	GLY	1687	25.901	-3.749	9.778	1.00	23.76
ATOM	1948	N	VAL	1688	24.928	-1.947	8.817	1.00	20.60
ATOM	1950	CA	VAL	1688	25.331	-1.009	9.877	1.00	22.34
ATOM	1951	CB	VAL	1688	25.020	0.481	9.488	1.00	20.94
ATOM	1952	CG1	VAL	1688	25.547	1.438	10.543	1.00	21.65
ATOM	1953	CG2	VAL	1688	25.675	0.832	8.160	1.00	22.71
ATOM	1954	C	VAL	1688	24.598	-1.400	11.182	1.00	22.71
ATOM	1955	O	VAL	1688	25.199	-1.479	12.255	1.00	22.78
ATOM	1956	N	LEU	1689	23.310	-1.706	11.082	1.00	22.81
ATOM	1958	CA	LEU	1689	22.534	-2.111	12.253	1.00	25.21
ATOM	1959	CB	LEU	1689	21.064	-2.357	11.866	1.00	25.78
ATOM	1960	CG	LEU	1689	20.006	-2.491	12.976	1.00	29.18
ATOM	1961	CD1	LEU	1689	18.643	-2.109	12.408	1.00	28.57
ATOM	1962	CD2	LEU	1689	19.959	-3.895	13.553	1.00	26.77
ATOM	1963	C	LEU	1689	23.158	-3.375	12.871	1.00	25.88
ATOM	1964	O	LEU	1689	23.249	-3.483	14.099	1.00	26.50
ATOM	1965	N	LEU	1690	23.588	-4.323	12.031	1.00	25.84
ATOM	1967	CA	LEU	1690	24.221	-5.544	12.523	1.00	24.43
ATOM	1968	CB	LEU	1690	24.669	-6.444	11.377	1.00	26.35
ATOM	1969	CG	LEU	1690	23.672	-7.309	10.604	1.00	26.57
ATOM	1970	CD1	LEU	1690	24.415	-7.962	9.446	1.00	26.33
ATOM	1971	CD2	LEU	1690	23.042	-8.380	11.502	1.00	24.66
ATOM	1972	C	LEU	1690	25.430	-5.168	13.349	1.00	25.22
ATOM	1973	O	LEU	1690	25.646	-5.706	14.435	1.00	24.84
ATOM	1974	N	TRP	1691	26.211	-4.227	12.826	1.00	26.92
ATOM	1976	CA	TRP	1691	27.405	-3.728	13.504	1.00	25.77
ATOM	1977	CB	TRP	1691	28.072	-2.659	12.631	1.00	24.82
ATOM	1978	CG	TRP	1691	29.394	-2.195	13.154	1.00	27.98

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ATOM	1979	CD2	TRP	1691	29.623	-1.104	14.056	1.00	26.95
ATOM	1980	CE2	TRP	1691	31.022	-1.015	14.259	1.00	27.64
ATOM	1981	CE3	TRP	1691	28.783	-0.191	14.708	1.00	26.28
ATOM	1982	CD1	TRP	1691	30.634	-2.715	12.856	1.00	28.38
ATOM	1983	NE1	TRP	1691	31.609	-2.009	13.518	1.00	29.56
ATOM	1985	CZ2	TRP	1691	31.599	-0.045	15.086	1.00	27.78
ATOM	1986	CZ3	TRP	1691	29.356	0.769	15.533	1.00	27.63
ATOM	1987	CH2	TRP	1691	30.753	0.835	15.713	1.00	30.68
ATOM	1988	C	TRP	1691	27.025	-3.147	14.876	1.00	26.38
ATOM	1989	O	TRP	1691	27.686	-3.414	15.883	1.00	24.82
ATOM	1990	N	GLU	1692	25.926	-2.393	14.916	1.00	27.62
ATOM	1992	CA	GLU	1692	25.442	-1.790	16.162	1.00	27.02
ATOM	1993	CB	GLU	1692	24.193	-0.963	15.919	1.00	29.27
ATOM	1994	CG	GLU	1692	24.345	0.236	15.028	1.00	24.77
ATOM	1995	CD	GLU	1692	23.046	0.992	14.962	1.00	25.98
ATOM	1996	OE1	GLU	1692	22.238	0.694	14.058	1.00	22.29
ATOM	1997	OE2	GLU	1692	22.803	1.837	15.850	1.00	25.12
ATOM	1998	C	GLU	1692	25.092	-2.856	17.191	1.00	27.88
ATOM	1999	O	GLU	1692	25.333	-2.673	18.379	1.00	30.18
ATOM	2000	N	ILE	1693	24.500	-3.956	16.734	1.00	26.65
ATOM	2002	CA	ILE	1693	24.118	-5.054	17.618	1.00	26.14
ATOM	2003	CB	ILE	1693	23.279	-6.144	16.858	1.00	25.37
ATOM	2004	CG2	ILE	1693	23.144	-7.445	17.704	1.00	21.48
ATOM	2005	CG1	ILE	1693	21.897	-5.563	16.496	1.00	24.80
ATOM	2006	CD1	ILE	1693	21.017	-6.479	15.642	1.00	22.40
ATOM	2007	C	ILE	1693	25.345	-5.698	18.239	1.00	27.17
ATOM	2008	O	ILE	1693	25.424	-5.864	19.452	1.00	27.30
ATOM	2009	N	PHE	1694	26.329	-6.017	17.414	1.00	29.98
ATOM	2011	CA	PHE	1694	27.518	-6.674	17.925	1.00	30.61
ATOM	2012	CB	PHE	1694	28.140	-7.556	16.843	1.00	28.30
ATOM	2013	CG	PHE	1694	27.197	-8.611	16.353	1.00	30.91
ATOM	2014	CD1	PHE	1694	26.627	-8.526	15.088	1.00	34.46
ATOM	2015	CD2	PHE	1694	26.743	-9.601	17.224	1.00	32.71
ATOM	2016	CE1	PHE	1694	25.622	-9.409	14.701	1.00	34.24
ATOM	2017	CE2	PHE	1694	25.737	-10.490	16.844	1.00	32.44
ATOM	2018	CZ	PHE	1694	25.170	-10.387	15.592	1.00	32.70
ATOM	2019	C	PHE	1694	28.512	-5.796	18.689	1.00	31.74
ATOM	2020	O	PHE	1694	29.469	-6.299	19.276	1.00	35.15
ATOM	2021	N	THR	1695	28.275	-4.489	18.698	1.00	31.12
ATOM	2023	CA	THR	1695	29.101	-3.575	19.473	1.00	29.96
ATOM	2024	CB	THR	1695	29.532	-2.351	18.657	1.00	28.09
ATOM	2025	OG1	THR	1695	28.373	-1.685	18.150	1.00	30.65
ATOM	2027	CG2	THR	1695	30.450	-2.767	17.510	1.00	23.37
ATOM	2028	C	THR	1695	28.240	-3.128	20.664	1.00	30.01
ATOM	2029	O	THR	1695	28.617	-2.233	21.427	1.00	31.14
ATOM	2030	N	LEU	1696	27.078	-3.766	20.797	1.00	27.96
ATOM	2032	CA	LEU	1696	26.113	-3.490	21.862	1.00	30.25
ATOM	2033	CB	LEU	1696	26.633	-3.985	23.216	1.00	33.54
ATOM	2034	CG	LEU	1696	26.899	-5.482	23.339	1.00	32.61
ATOM	2035	CD1	LEU	1696	27.473	-5.777	24.711	1.00	33.54
ATOM	2036	CD2	LEU	1696	25.602	-6.233	23.126	1.00	36.37
ATOM	2037	C	LEU	1696	25.717	-2.031	21.958	1.00	28.19
ATOM	2038	O	LEU	1696	25.792	-1.431	23.018	1.00	29.18
ATOM	2039	N	GLY	1697	25.251	-1.472	20.853	1.00	28.24

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ATOM	2041	CA	GLY	1697	24.851	-0.082	20.858	1.00	28.29
ATOM	2042	C	GLY	1697	25.990	0.845	20.499	1.00	27.68
ATOM	2043	O	GLY	1697	25.960	2.022	20.846	1.00	29.79
ATOM	2044	N	GLY	1698	26.986	0.324	19.790	1.00	29.23
ATOM	2046	CA	GLY	1698	28.115	1.143	19.396	1.00	30.79
ATOM	2047	C	GLY	1698	27.743	2.212	18.388	1.00	32.38
ATOM	2048	O	GLY	1698	26.817	2.044	17.601	1.00	33.26
ATOM	2049	N	SER	1699	28.480	3.314	18.411	1.00	30.81
ATOM	2051	CA	SER	1699	28.268	4.437	17.510	1.00	32.03
ATOM	2052	CB	SER	1699	28.528	5.728	18.288	1.00	34.81
ATOM	2053	OG	SER	1699	28.559	6.862	17.440	1.00	40.03
ATOM	2055	C	SER	1699	29.198	4.325	16.282	1.00	32.20
ATOM	2056	O	SER	1699	30.428	4.325	16.408	1.00	31.67
ATOM	2057	N	PRO	1700	28.620	4.148	15.082	1.00	32.62
ATOM	2058	CD	PRO	1700	27.178	4.142	14.773	1.00	34.19
ATOM	2059	CA	PRO	1700	29.422	4.028	13.856	1.00	31.76
ATOM	2060	CB	PRO	1700	28.357	3.830	12.759	1.00	32.04
ATOM	2061	CG	PRO	1700	27.145	3.351	13.502	1.00	33.17
ATOM	2062	C	PRO	1700	30.214	5.309	13.609	1.00	28.70
ATOM	2063	O	PRO	1700	29.715	6.391	13.871	1.00	28.57
ATOM	2064	N	TYR	1701	31.459	5.181	13.164	1.00	28.61
ATOM	2066	CA	TYR	1701	32.311	6.338	12.870	1.00	29.92
ATOM	2067	CB	TYR	1701	31.920	6.946	11.510	1.00	30.15
ATOM	2068	CG	TYR	1701	31.965	5.994	10.339	1.00	36.17
ATOM	2069	CD1	TYR	1701	30.799	5.630	9.664	1.00	39.26
ATOM	2070	CE1	TYR	1701	30.839	4.767	8.571	1.00	41.51
ATOM	2071	CD2	TYR	1701	33.176	5.467	9.893	1.00	37.48
ATOM	2072	CE2	TYR	1701	33.229	4.607	8.805	1.00	42.94
ATOM	2073	CZ	TYR	1701	32.059	4.263	8.146	1.00	45.72
ATOM	2074	OH	TYR	1701	32.110	3.431	7.043	1.00	53.99
ATOM	2076	C	TYR	1701	32.279	7.448	13.941	1.00	31.09
ATOM	2077	O	TYR	1701	31.935	8.592	13.649	1.00	31.93
ATOM	2078	N	PRO	1702	32.649	7.135	15.189	1.00	34.66
ATOM	2079	CD	PRO	1702	33.212	5.879	15.708	1.00	36.83
ATOM	2080	CA	PRO	1702	32.631	8.173	16.231	1.00	33.54
ATOM	2081	CB	PRO	1702	33.116	7.432	17.479	1.00	32.18
ATOM	2082	CG	PRO	1702	32.903	6.001	17.175	1.00	40.82
ATOM	2083	C	PRO	1702	33.628	9.274	15.883	1.00	34.78
ATOM	2084	O	PRO	1702	34.750	8.981	15.455	1.00	33.97
ATOM	2085	N	GLY	1703	33.220	10.528	16.074	1.00	36.45
ATOM	2087	CA	GLY	1703	34.085	11.667	15.788	1.00	34.40
ATOM	2088	C	GLY	1703	34.245	12.006	14.317	1.00	34.34
ATOM	2089	O	GLY	1703	34.977	12.933	13.969	1.00	34.20
ATOM	2090	N	VAL	1704	33.552	11.275	13.445	1.00	35.02
ATOM	2092	CA	VAL	1704	33.641	11.512	12.007	1.00	32.77
ATOM	2093	CB	VAL	1704	33.614	10.176	11.221	1.00	31.32
ATOM	2094	CG1	VAL	1704	33.628	10.435	9.709	1.00	31.46
ATOM	2095	CG2	VAL	1704	34.796	9.297	11.637	1.00	27.62
ATOM	2096	C	VAL	1704	32.510	12.410	11.513	1.00	33.35
ATOM	2097	O	VAL	1704	31.337	12.070	11.640	1.00	33.94
ATOM	2098	N	PRO	1705	32.849	13.589	10.974	1.00	32.43
ATOM	2099	CD	PRO	1705	34.181	14.221	10.949	1.00	32.77
ATOM	2100	CA	PRO	1705	31.826	14.505	10.472	1.00	33.61
ATOM	2101	CB	PRO	1705	32.545	15.853	10.509	1.00	33.21

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ATOM	2102	CG	PRO	1705	33.935	15.482	10.141	1.00	35.53
ATOM	2103	C	PRO	1705	31.395	14.138	9.052	1.00	33.91
ATOM	2104	O	PRO	1705	32.113	13.409	8.354	1.00	32.65
ATOM	2105	N	VAL	1706	30.255	14.684	8.619	1.00	33.82
ATOM	2107	CA	VAL	1706	29.689	14.447	7.280	1.00	33.97
ATOM	2108	CB	VAL	1706	28.617	15.513	6.943	1.00	37.41
ATOM	2109	CG1	VAL	1706	28.045	15.282	5.556	1.00	41.12
ATOM	2110	CG2	VAL	1706	27.507	15.484	7.971	1.00	38.89
ATOM	2111	C	VAL	1706	30.712	14.428	6.135	1.00	32.32
ATOM	2112	O	VAL	1706	30.819	13.450	5.398	1.00	32.58
ATOM	2113	N	GLU	1707	31.477	15.504	6.004	1.00	31.15
ATOM	2115	CA	GLU	1707	32.478	15.630	4.956	1.00	29.82
ATOM	2116	CB	GLU	1707	33.172	16.989	5.048	1.00	30.05
ATOM	2117	C	GLU	1707	33.531	14.541	4.959	1.00	28.52
ATOM	2118	O	GLU	1707	33.995	14.134	3.896	1.00	30.85
ATOM	2119	N	GLU	1708	33.958	14.110	6.143	1.00	28.70
ATOM	2121	CA	GLU	1708	34.978	13.073	6.235	1.00	29.50
ATOM	2122	CB	GLU	1708	35.590	13.010	7.641	1.00	31.28
ATOM	2123	CG	GLU	1708	36.281	14.289	8.103	1.00	41.63
ATOM	2124	CD	GLU	1708	37.454	14.718	7.237	1.00	49.91
ATOM	2125	OE1	GLU	1708	38.020	13.876	6.498	1.00	53.57
ATOM	2126	OE2	GLU	1708	37.821	15.916	7.308	1.00	58.45
ATOM	2127	C	GLU	1708	34.365	11.730	5.878	1.00	30.00
ATOM	2128	O	GLU	1708	35.016	10.874	5.257	1.00	28.43
ATOM	2129	N	LEU	1709	33.103	11.559	6.257	1.00	30.08
ATOM	2131	CA	LEU	1709	32.392	10.324	5.964	1.00	29.19
ATOM	2132	CB	LEU	1709	30.995	10.347	6.592	1.00	28.97
ATOM	2133	CG	LEU	1709	30.109	9.186	6.137	1.00	30.66
ATOM	2134	CD1	LEU	1709	30.664	7.866	6.659	1.00	29.24
ATOM	2135	CD2	LEU	1709	28.684	9.403	6.593	1.00	29.29
ATOM	2136	C	LEU	1709	32.294	10.130	4.449	1.00	28.26
ATOM	2137	O	LEU	1709	32.450	9.011	3.948	1.00	28.86
ATOM	2138	N	PHE	1710	32.016	11.220	3.735	1.00	26.86
ATOM	2140	CA	PHE	1710	31.903	11.192	2.285	1.00	28.86
ATOM	2141	CB	PHE	1710	31.632	12.593	1.743	1.00	31.88
ATOM	2142	CG	PHE	1710	30.249	13.095	2.014	1.00	37.62
ATOM	2143	CD1	PHE	1710	29.265	12.247	2.509	1.00	42.63
ATOM	2144	CD2	PHE	1710	29.931	14.424	1.792	1.00	43.53
ATOM	2145	CE1	PHE	1710	27.977	12.718	2.783	1.00	45.99
ATOM	2146	CE2	PHE	1710	28.648	14.905	2.061	1.00	46.25
ATOM	2147	CZ	PHE	1710	27.670	14.045	2.559	1.00	44.45
ATOM	2148	C	PHE	1710	33.193	10.660	1.681	1.00	30.42
ATOM	2149	O	PHE	1710	33.174	9.807	0.792	1.00	29.01
ATOM	2150	N	LYS	1711	34.309	11.152	2.212	1.00	30.64
ATOM	2152	CA	LYS	1711	35.650	10.762	1.786	1.00	32.89
ATOM	2153	CB	LYS	1711	36.670	11.655	2.502	1.00	37.91
ATOM	2154	CG	LYS	1711	38.108	11.479	2.088	1.00	42.99
ATOM	2155	CD	LYS	1711	38.976	12.528	2.752	1.00	47.45
ATOM	2156	CE	LYS	1711	40.380	12.505	2.182	1.00	52.35
ATOM	2157	NZ	LYS	1711	41.104	11.272	2.587	1.00	58.47
ATOM	2161	C	LYS	1711	35.913	9.273	2.071	1.00	32.23
ATOM	2162	O	LYS	1711	36.445	8.559	1.216	1.00	30.79
ATOM	2163	N	LEU	1712	35.533	8.807	3.264	1.00	31.37
ATOM	2165	CA	LEU	1712	35.704	7.399	3.630	1.00	29.46

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ATOM	2166	CB	LEU	1712	35.220	7.117	5.065	1.00	28.57
ATOM	2167	CG	LEU	1712	36.045	7.662	6.242	1.00	30.18
ATOM	2168	CD1	LEU	1712	35.395	7.349	7.569	1.00	26.92
ATOM	2169	CD2	LEU	1712	37.452	7.083	6.210	1.00	30.88
ATOM	2170	C	LEU	1712	34.922	6.539	2.651	1.00	28.99
ATOM	2171	O	LEU	1712	35.438	5.551	2.136	1.00	30.73
ATOM	2172	N	LEU	1713	33.675	6.915	2.388	1.00	30.13
ATOM	2174	CA	LEU	1713	32.851	6.158	1.456	1.00	32.10
ATOM	2175	CB	LEU	1713	31.411	6.685	1.443	1.00	35.23
ATOM	2176	CG	LEU	1713	30.612	6.292	2.691	1.00	37.47
ATOM	2177	CD1	LEU	1713	29.265	6.982	2.720	1.00	40.85
ATOM	2178	CD2	LEU	1713	30.447	4.788	2.723	1.00	39.61
ATOM	2179	C	LEU	1713	33.441	6.147	0.047	1.00	32.70
ATOM	2180	O	LEU	1713	33.548	5.090	-0.578	1.00	31.86
ATOM	2181	N	LYS	1714	33.859	7.309	-0.444	1.00	32.42
ATOM	2183	CA	LYS	1714	34.440	7.387	-1.776	1.00	32.56
ATOM	2184	CB	LYS	1714	34.826	8.824	-2.112	1.00	33.02
ATOM	2185	CG	LYS	1714	33.640	9.736	-2.297	1.00	35.56
ATOM	2186	CD	LYS	1714	32.736	9.235	-3.396	1.00	37.94
ATOM	2187	CE	LYS	1714	31.635	10.246	-3.682	1.00	42.57
ATOM	2188	NZ	LYS	1714	30.727	9.805	-4.779	1.00	47.40
ATOM	2192	C	LYS	1714	35.664	6.488	-1.885	1.00	35.36
ATOM	2193	O	LYS	1714	35.927	5.898	-2.937	1.00	36.68
ATOM	2194	N	GLU	1715	36.376	6.338	-0.775	1.00	34.51
ATOM	2196	CA	GLU	1715	37.577	5.527	-0.749	1.00	35.31
ATOM	2197	CB	GLU	1715	38.566	6.125	0.250	1.00	37.07
ATOM	2198	CG	GLU	1715	38.967	7.537	-0.163	1.00	43.62
ATOM	2199	CD	GLU	1715	39.735	8.310	0.893	1.00	49.75
ATOM	2200	OE1	GLU	1715	39.906	7.814	2.029	1.00	49.71
ATOM	2201	OE2	GLU	1715	40.163	9.442	0.572	1.00	55.13
ATOM	2202	C	GLU	1715	37.321	4.048	-0.487	1.00	34.08
ATOM	2203	O	GLU	1715	38.259	3.260	-0.438	1.00	34.82
ATOM	2204	N	GLY	1716	36.049	3.674	-0.366	1.00	31.53
ATOM	2206	CA	GLY	1716	35.695	2.288	-0.133	1.00	27.58
ATOM	2207	C	GLY	1716	35.966	1.765	1.262	1.00	28.60
ATOM	2208	O	GLY	1716	36.069	0.560	1.464	1.00	27.81
ATOM	2209	N	HIS	1717	36.062	2.663	2.236	1.00	29.10
ATOM	2211	CA	HIS	1717	36.319	2.263	3.617	1.00	29.30
ATOM	2212	CB	HIS	1717	36.501	3.510	4.486	1.00	30.54
ATOM	2213	CG	HIS	1717	36.788	3.213	5.930	1.00	32.88
ATOM	2214	CD2	HIS	1717	37.961	3.023	6.586	1.00	32.21
ATOM	2215	ND1	HIS	1717	35.798	3.108	6.881	1.00	34.22
ATOM	2217	CE1	HIS	1717	36.342	2.865	8.061	1.00	31.51
ATOM	2218	NE2	HIS	1717	37.651	2.809	7.907	1.00	31.94
ATOM	2220	C	HIS	1717	35.180	1.416	4.183	1.00	28.42
ATOM	2221	O	HIS	1717	34.017	1.666	3.885	1.00	30.71
ATOM	2222	N	ARG	1718	35.526	0.450	5.028	1.00	27.75
ATOM	2224	CA	ARG	1718	34.559	-0.423	5.688	1.00	27.58
ATOM	2225	CB	ARG	1718	34.562	-1.813	5.048	1.00	29.07
ATOM	2226	CG	ARG	1718	34.078	-1.860	3.597	1.00	28.39
ATOM	2227	CD	ARG	1718	32.609	-1.412	3.475	1.00	27.64
ATOM	2228	NE	ARG	1718	32.091	-1.467	2.096	1.00	24.37
ATOM	2230	CZ	ARG	1718	32.173	-0.476	1.210	1.00	24.26
ATOM	2231	NH1	ARG	1718	32.768	0.668	1.532	1.00	23.98

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ATOM	2234	NH2	ARG	1718	31.595	-0.603	0.019	1.00	21.60
ATOM	2237	C	ARG	1718	35.005	-0.521	7.148	1.00	30.11
ATOM	2238	O	ARG	1718	36.201	-0.623	7.428	1.00	30.60
ATOM	2239	N	MET	1719	34.056	-0.430	8.074	1.00	30.69
ATOM	2241	CA	MET	1719	34.350	-0.490	9.501	1.00	31.77
ATOM	2242	CB	MET	1719	33.072	-0.302	10.335	1.00	34.56
ATOM	2243	CG	MET	1719	32.408	1.060	10.194	1.00	36.71
ATOM	2244	SD	MET	1719	31.015	1.307	11.314	1.00	38.66
ATOM	2245	CE	MET	1719	29.797	0.338	10.544	1.00	36.99
ATOM	2246	C	MET	1719	34.998	-1.810	9.854	1.00	30.20
ATOM	2247	O	MET	1719	34.802	-2.802	9.169	1.00	31.41
ATOM	2248	N	ASP	1720	35.778	-1.809	10.926	1.00	32.49
ATOM	2250	CA	ASP	1720	36.473	-3.008	11.385	1.00	33.60
ATOM	2251	CB	ASP	1720	37.593	-2.630	12.358	1.00	37.65
ATOM	2252	CG	ASP	1720	38.628	-1.688	11.747	1.00	44.69
ATOM	2253	OD1	ASP	1720	38.442	-1.223	10.596	1.00	50.97
ATOM	2254	OD2	ASP	1720	39.632	-1.398	12.443	1.00	48.67
ATOM	2255	C	ASP	1720	35.524	-3.977	12.079	1.00	31.26
ATOM	2256	O	ASP	1720	34.466	-3.581	12.561	1.00	32.69
ATOM	2257	N	LYS	1721	35.943	-5.231	12.191	1.00	32.76
ATOM	2259	CA	LYS	1721	35.133	-6.261	12.825	1.00	32.28
ATOM	2260	CB	LYS	1721	35.726	-7.649	12.575	1.00	33.63
ATOM	2261	CG	LYS	1721	34.854	-8.773	13.125	1.00	35.68
ATOM	2262	CD	LYS	1721	35.392	-10.126	12.784	1.00	36.22
ATOM	2263	CE	LYS	1721	36.054	-10.749	13.988	1.00	42.65
ATOM	2264	NZ	LYS	1721	36.354	-12.189	13.756	1.00	46.15
ATOM	2268	C	LYS	1721	35.039	-6.051	14.315	1.00	35.55
ATOM	2269	O	LYS	1721	36.064	-5.926	14.986	1.00	37.78
ATOM	2270	N	PRO	1722	33.807	-6.017	14.861	1.00	36.91
ATOM	2271	CD	PRO	1722	32.504	-6.105	14.179	1.00	34.43
ATOM	2272	CA	PRO	1722	33.630	-5.827	16.305	1.00	37.77
ATOM	2273	CB	PRO	1722	32.107	-5.846	16.465	1.00	36.32
ATOM	2274	CG	PRO	1722	31.603	-5.375	15.122	1.00	34.53
ATOM	2275	C	PRO	1722	34.246	-7.026	17.023	1.00	39.31
ATOM	2276	O	PRO	1722	34.274	-8.136	16.477	1.00	38.78
ATOM	2277	N	SER	1723	34.777	-6.820	18.222	1.00	42.72
ATOM	2279	CA	SER	1723	35.336	-7.954	18.940	1.00	45.01
ATOM	2280	CB	SER	1723	36.152	-7.508	20.160	1.00	46.88
ATOM	2281	OG	SER	1723	35.327	-7.027	21.208	1.00	53.47
ATOM	2283	C	SER	1723	34.088	-8.731	19.359	1.00	46.67
ATOM	2284	O	SER	1723	32.982	-8.172	19.417	1.00	46.21
ATOM	2285	N	ASN	1724	34.237	-10.025	19.590	1.00	47.80
ATOM	2287	CA	ASN	1724	33.092	-10.826	19.999	1.00	52.78
ATOM	2288	CB	ASN	1724	32.559	-10.319	21.355	1.00	57.86
ATOM	2289	CG	ASN	1724	33.679	-10.091	22.370	1.00	61.99
ATOM	2290	OD1	ASN	1724	34.531	-10.959	22.585	1.00	63.17
ATOM	2291	ND2	ASN	1724	33.712	-8.899	22.953	1.00	63.56
ATOM	2294	C	ASN	1724	32.015	-10.779	18.893	1.00	51.43
ATOM	2295	O	ASN	1724	30.859	-10.423	19.108	1.00	51.56
ATOM	2296	N	CYS	1725	32.454	-11.087	17.683	1.00	48.91
ATOM	2298	CA	CYS	1725	31.600	-11.136	16.508	1.00	45.62
ATOM	2299	CB	CYS	1725	31.526	-9.771	15.811	1.00	44.83
ATOM	2300	SG	CYS	1725	30.693	-9.816	14.194	1.00	41.83
ATOM	2301	C	CYS	1725	32.341	-12.135	15.640	1.00	42.30

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ATOM	2302	O	CYS	1725	33.566	-12.045	15.493	1.00	44.63
ATOM	2303	N	THR	1726	31.627	-13.134	15.141	1.00	37.46
ATOM	2305	CA	THR	1726	32.259	-14.153	14.320	1.00	35.29
ATOM	2306	CB	THR	1726	31.339	-15.367	14.132	1.00	33.44
ATOM	2307	OG1	THR	1726	30.109	-14.952	13.523	1.00	34.77
ATOM	2309	CG2	THR	1726	31.070	-16.019	15.454	1.00	30.22
ATOM	2310	C	THR	1726	32.668	-13.622	12.963	1.00	33.53
ATOM	2311	O	THR	1726	32.158	-12.593	12.518	1.00	32.93
ATOM	2312	N	ASN	1727	33.619	-14.294	12.319	1.00	32.72
ATOM	2314	CA	ASN	1727	34.030	-13.867	10.983	1.00	35.91
ATOM	2315	CB	ASN	1727	35.166	-14.724	10.422	1.00	40.64
ATOM	2316	CG	ASN	1727	36.463	-14.533	11.168	1.00	46.52
ATOM	2317	OD1	ASN	1727	37.047	-13.453	11.158	1.00	49.98
ATOM	2318	ND2	ASN	1727	36.931	-15.592	11.814	1.00	49.04
ATOM	2321	C	ASN	1727	32.824	-14.006	10.058	1.00	34.27
ATOM	2322	O	ASN	1727	32.681	-13.236	9.116	1.00	32.96
ATOM	2323	N	GLU	1728	31.969	-14.997	10.326	1.00	32.49
ATOM	2325	CA	GLU	1728	30.778	-15.235	9.510	1.00	31.99
ATOM	2326	CB	GLU	1728	30.064	-16.504	9.975	1.00	34.15
ATOM	2327	CG	GLU	1728	28.836	-16.866	9.156	1.00	35.63
ATOM	2328	CD	GLU	1728	28.187	-18.169	9.608	1.00	39.72
ATOM	2329	OE1	GLU	1728	28.200	-18.463	10.824	1.00	42.25
ATOM	2330	OE2	GLU	1728	27.654	-18.896	8.742	1.00	39.87
ATOM	2331	C	GLU	1728	29.814	-14.049	9.549	1.00	30.76
ATOM	2332	O	GLU	1728	29.309	-13.602	8.512	1.00	29.58
ATOM	2333	N	LEU	1729	29.559	-13.544	10.750	1.00	30.01
ATOM	2335	CA	LEU	1729	28.670	-12.408	10.911	1.00	30.21
ATOM	2336	CB	LEU	1729	28.225	-12.272	12.364	1.00	30.13
ATOM	2337	CG	LEU	1729	27.208	-13.350	12.748	1.00	33.61
ATOM	2338	CD1	LEU	1729	27.119	-13.483	14.262	1.00	33.71
ATOM	2339	CD2	LEU	1729	25.844	-13.021	12.139	1.00	30.31
ATOM	2340	C	LEU	1729	29.316	-11.133	10.390	1.00	30.26
ATOM	2341	O	LEU	1729	28.619	-10.229	9.938	1.00	28.89
ATOM	2342	N	TYR	1730	30.648	-11.063	10.435	1.00	28.91
ATOM	2344	CA	TYR	1730	31.343	-9.893	9.912	1.00	28.91
ATOM	2345	CB	TYR	1730	32.804	-9.861	10.359	1.00	29.09
ATOM	2346	CG	TYR	1730	33.537	-8.639	9.857	1.00	30.15
ATOM	2347	CD1	TYR	1730	33.037	-7.358	10.103	1.00	29.97
ATOM	2348	CE1	TYR	1730	33.688	-6.227	9.626	1.00	28.99
ATOM	2349	CD2	TYR	1730	34.716	-8.757	9.119	1.00	29.24
ATOM	2350	CE2	TYR	1730	35.386	-7.620	8.632	1.00	28.25
ATOM	2351	CZ	TYR	1730	34.861	-6.362	8.889	1.00	28.41
ATOM	2352	OH	TYR	1730	35.485	-5.227	8.405	1.00	31.64
ATOM	2354	C	TYR	1730	31.260	-9.943	8.379	1.00	27.10
ATOM	2355	O	TYR	1730	31.078	-8.920	7.726	1.00	27.46
ATOM	2356	N	MET	1731	31.390	-11.138	7.813	1.00	26.68
ATOM	2358	CA	MET	1731	31.298	-11.315	6.372	1.00	28.68
ATOM	2359	CB	MET	1731	31.526	-12.778	5.989	1.00	35.43
ATOM	2360	CG	MET	1731	31.158	-13.087	4.545	1.00	46.19
ATOM	2361	SD	MET	1731	31.441	-14.804	4.064	1.00	60.10
ATOM	2362	CE	MET	1731	32.603	-14.550	2.678	1.00	58.31
ATOM	2363	C	MET	1731	29.917	-10.858	5.912	1.00	27.42
ATOM	2364	O	MET	1731	29.782	-10.227	4.871	1.00	30.80
ATOM	2365	N	MET	1732	28.893	-11.191	6.688	1.00	28.53

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ATOM	2367	CA	MET	1732	27.522	-10.777	6.389	1.00	26.47
ATOM	2368	CB	MET	1732	26.562	-11.308	7.458	1.00	25.79
ATOM	2369	CG	MET	1732	25.116	-10.838	7.274	1.00	26.01
ATOM	2370	SD	MET	1732	24.004	-11.550	8.469	1.00	26.22
ATOM	2371	CE	MET	1732	23.787	-13.195	7.783	1.00	23.74
ATOM	2372	C	MET	1732	27.445	-9.243	6.319	1.00	25.15
ATOM	2373	O	MET	1732	26.886	-8.691	5.379	1.00	25.41
ATOM	2374	N	MET	1733	28.024	-8.564	7.308	1.00	26.48
ATOM	2376	CA	MET	1733	28.057	-7.104	7.331	1.00	27.09
ATOM	2377	CB	MET	1733	28.903	-6.594	8.488	1.00	25.91
ATOM	2378	CG	MET	1733	28.235	-6.556	9.824	1.00	31.64
ATOM	2379	SD	MET	1733	29.442	-6.111	11.094	1.00	29.59
ATOM	2380	CE	MET	1733	28.886	-7.126	12.420	1.00	28.14
ATOM	2381	C	MET	1733	28.720	-6.613	6.056	1.00	28.43
ATOM	2382	O	MET	1733	28.185	-5.753	5.372	1.00	31.37
ATOM	2383	N	ARG	1734	29.891	-7.169	5.747	1.00	28.57
ATOM	2385	CA	ARG	1734	30.642	-6.783	4.551	1.00	27.00
ATOM	2386	CB	ARG	1734	32.007	-7.488	4.510	1.00	25.98
ATOM	2387	CG	ARG	1734	32.927	-7.154	5.707	1.00	28.13
ATOM	2388	CD	ARG	1734	33.229	-5.672	5.765	1.00	29.97
ATOM	2389	NE	ARG	1734	33.922	-5.256	4.553	1.00	40.49
ATOM	2391	CZ	ARG	1734	35.238	-5.361	4.363	1.00	43.95
ATOM	2392	NH1	ARG	1734	36.023	-5.853	5.318	1.00	41.81
ATOM	2395	NH2	ARG	1734	35.760	-5.048	3.184	1.00	46.20
ATOM	2398	C	ARG	1734	29.859	-7.037	3.268	1.00	24.57
ATOM	2399	O	ARG	1734	29.992	-6.290	2.314	1.00	24.94
ATOM	2400	N	ASP	1735	29.071	-8.107	3.235	1.00	24.79
ATOM	2402	CA	ASP	1735	28.254	-8.420	2.061	1.00	23.88
ATOM	2403	CB	ASP	1735	27.669	-9.830	2.150	1.00	25.95
ATOM	2404	CG	ASP	1735	28.724	-10.913	2.024	1.00	27.60
ATOM	2405	OD1	ASP	1735	29.842	-10.632	1.529	1.00	27.75
ATOM	2406	OD2	ASP	1735	28.432	-12.051	2.430	1.00	28.90
ATOM	2407	C	ASP	1735	27.139	-7.396	1.941	1.00	22.61
ATOM	2408	O	ASP	1735	26.777	-6.996	0.833	1.00	22.66
ATOM	2409	N	CYS	1736	26.611	-6.965	3.085	1.00	20.61
ATOM	2411	CA	CYS	1736	25.561	-5.952	3.109	1.00	23.63
ATOM	2412	CB	CYS	1736	25.007	-5.767	4.534	1.00	21.98
ATOM	2413	SG	CYS	1736	23.934	-7.126	5.111	1.00	22.95
ATOM	2414	C	CYS	1736	26.129	-4.633	2.599	1.00	23.62
ATOM	2415	O	CYS	1736	25.403	-3.797	2.047	1.00	22.15
ATOM	2416	N	TRP	1737	27.438	-4.461	2.775	1.00	24.37
ATOM	2418	CA	TRP	1737	28.123	-3.247	2.342	1.00	23.77
ATOM	2419	CB	TRP	1737	29.162	-2.810	3.371	1.00	19.38
ATOM	2420	CG	TRP	1737	28.601	-2.520	4.718	1.00	21.62
ATOM	2421	CD2	TRP	1737	29.268	-2.688	5.971	1.00	24.81
ATOM	2422	CE2	TRP	1737	28.371	-2.278	6.980	1.00	25.95
ATOM	2423	CE3	TRP	1737	30.534	-3.165	6.340	1.00	29.02
ATOM	2424	CD1	TRP	1737	27.359	-2.024	5.007	1.00	23.21
ATOM	2425	NE1	TRP	1737	27.213	-1.876	6.362	1.00	21.80
ATOM	2427	CZ2	TRP	1737	28.710	-2.305	8.347	1.00	26.68
ATOM	2428	CZ3	TRP	1737	30.873	-3.198	7.699	1.00	31.06
ATOM	2429	CH2	TRP	1737	29.959	-2.774	8.685	1.00	30.18
ATOM	2430	C	TRP	1737	28.788	-3.372	0.978	1.00	24.88
ATOM	2431	O	TRP	1737	29.737	-2.646	0.689	1.00	25.11

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ATOM	2432	N	HIS	1738	28.303	-4.278	0.132	1.00	25.27
ATOM	2434	CA	HIS	1738	28.888	-4.406	-1.191	1.00	24.27
ATOM	2435	CB	HIS	1738	28.280	-5.573	-1.986	1.00	25.24
ATOM	2436	CG	HIS	1738	29.179	-6.073	-3.081	1.00	26.28
ATOM	2437	CD2	HIS	1738	29.727	-5.437	-4.147	1.00	25.67
ATOM	2438	ND1	HIS	1738	29.697	-7.352	-3.098	1.00	27.55
ATOM	2440	CE1	HIS	1738	30.528	-7.478	-4.117	1.00	27.51
ATOM	2441	NE2	HIS	1738	30.564	-6.329	-4.770	1.00	30.93
ATOM	2443	C	HIS	1738	28.715	-3.087	-1.953	1.00	25.59
ATOM	2444	O	HIS	1738	27.659	-2.451	-1.905	1.00	22.01
ATOM	2445	N	ALA	1739	29.784	-2.651	-2.612	1.00	23.84
ATOM	2447	CA	ALA	1739	29.759	-1.418	-3.388	1.00	24.93
ATOM	2448	CB	ALA	1739	31.131	-1.177	-4.024	1.00	26.39
ATOM	2449	C	ALA	1739	28.671	-1.508	-4.462	1.00	25.35
ATOM	2450	O	ALA	1739	27.963	-0.535	-4.727	1.00	28.20
ATOM	2451	N	VAL	1740	28.543	-2.680	-5.073	1.00	22.68
ATOM	2453	CA	VAL	1740	27.528	-2.904	-6.101	1.00	26.46
ATOM	2454	CB	VAL	1740	27.995	-3.968	-7.117	1.00	29.70
ATOM	2455	CG1	VAL	1740	27.063	-4.003	-8.334	1.00	26.01
ATOM	2456	CG2	VAL	1740	29.433	-3.686	-7.537	1.00	31.22
ATOM	2457	C	VAL	1740	26.213	-3.358	-5.443	1.00	25.07
ATOM	2458	O	VAL	1740	26.138	-4.474	-4.903	1.00	23.55
ATOM	2459	N	PRO	1741	25.155	-2.519	-5.514	1.00	25.30
ATOM	2460	CD	PRO	1741	25.133	-1.190	-6.153	1.00	22.43
ATOM	2461	CA	PRO	1741	23.844	-2.833	-4.921	1.00	24.09
ATOM	2462	CB	PRO	1741	22.962	-1.675	-5.402	1.00	23.12
ATOM	2463	CG	PRO	1741	23.928	-0.527	-5.491	1.00	22.04
ATOM	2464	C	PRO	1741	23.272	-4.191	-5.313	1.00	22.18
ATOM	2465	O	PRO	1741	22.727	-4.900	-4.466	1.00	21.23
ATOM	2466	N	SER	1742	23.437	-4.570	-6.580	1.00	23.87
ATOM	2468	CA	SER	1742	22.928	-5.847	-7.088	1.00	24.36
ATOM	2469	CB	SER	1742	23.071	-5.907	-8.612	1.00	27.39
ATOM	2470	OG	SER	1742	24.436	-6.025	-8.986	1.00	29.25
ATOM	2472	C	SER	1742	23.636	-7.058	-6.488	1.00	23.96
ATOM	2473	O	SER	1742	23.145	-8.179	-6.575	1.00	24.30
ATOM	2474	N	GLN	1743	24.810	-6.839	-5.915	1.00	24.39
ATOM	2476	CA	GLN	1743	25.558	-7.934	-5.345	1.00	23.15
ATOM	2477	CB	GLN	1743	27.046	-7.755	-5.638	1.00	23.83
ATOM	2478	CG	GLN	1743	27.359	-7.784	-7.126	1.00	22.84
ATOM	2479	CD	GLN	1743	26.816	-9.036	-7.808	1.00	24.20
ATOM	2480	OE1	GLN	1743	27.318	-10.135	-7.590	1.00	21.50
ATOM	2481	NE2	GLN	1743	25.775	-8.871	-8.628	1.00	22.45
ATOM	2484	C	GLN	1743	25.309	-8.171	-3.868	1.00	23.12
ATOM	2485	O	GLN	1743	25.816	-9.135	-3.317	1.00	24.96
ATOM	2486	N	ARG	1744	24.557	-7.280	-3.225	1.00	23.67
ATOM	2488	CA	ARG	1744	24.242	-7.424	-1.806	1.00	22.11
ATOM	2489	CB	ARG	1744	23.699	-6.110	-1.231	1.00	19.70
ATOM	2490	CG	ARG	1744	24.672	-4.959	-1.338	1.00	21.26
ATOM	2491	CD	ARG	1744	24.049	-3.640	-0.890	1.00	20.68
ATOM	2492	NE	ARG	1744	24.923	-2.552	-1.305	1.00	25.21
ATOM	2494	CZ	ARG	1744	24.540	-1.313	-1.583	1.00	24.30
ATOM	2495	NH1	ARG	1744	23.257	-0.955	-1.481	1.00	22.04
ATOM	2498	NH2	ARG	1744	25.450	-0.448	-2.036	1.00	21.29
ATOM	2501	C	ARG	1744	23.184	-8.505	-1.640	1.00	22.53

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ATOM	2502	O	ARG	1744	22.437	-8.800	-2.588	1.00	23.08
ATOM	2503	N	PRO	1745	23.162	-9.170	-0.467	1.00	20.76
ATOM	2504	CD	PRO	1745	24.087	-9.078	0.681	1.00	21.71
ATOM	2505	CA	PRO	1745	22.160	-10.207	-0.243	1.00	22.34
ATOM	2506	CB	PRO	1745	22.632	-10.859	1.057	1.00	20.58
ATOM	2507	CG	PRO	1745	23.298	-9.727	1.783	1.00	20.36
ATOM	2508	C	PRO	1745	20.814	-9.512	-0.048	1.00	23.62
ATOM	2509	O	PRO	1745	20.759	-8.318	0.255	1.00	25.29
ATOM	2510	N	THR	1746	19.731	-10.235	-0.275	1.00	23.39
ATOM	2512	CA	THR	1746	18.404	-9.675	-0.080	1.00	22.77
ATOM	2513	CB	THR	1746	17.386	-10.368	-1.004	1.00	23.24
ATOM	2514	OG1	THR	1746	17.409	-11.783	-0.763	1.00	23.11
ATOM	2516	CG2	THR	1746	17.724	-10.103	-2.475	1.00	24.96
ATOM	2517	C	THR	1746	18.009	-9.954	1.365	1.00	24.98
ATOM	2518	O	THR	1746	18.664	-10.758	2.043	1.00	24.30
ATOM	2519	N	PHE	1747	16.944	-9.318	1.853	1.00	24.95
ATOM	2521	CA	PHE	1747	16.501	-9.596	3.221	1.00	25.16
ATOM	2522	CB	PHE	1747	15.395	-8.628	3.661	1.00	23.64
ATOM	2523	CG	PHE	1747	15.916	-7.283	4.089	1.00	24.34
ATOM	2524	CD1	PHE	1747	16.715	-7.167	5.226	1.00	21.21
ATOM	2525	CD2	PHE	1747	15.649	-6.137	3.334	1.00	21.42
ATOM	2526	CE1	PHE	1747	17.252	-5.932	5.597	1.00	20.99
ATOM	2527	CE2	PHE	1747	16.178	-4.907	3.699	1.00	20.36
ATOM	2528	CZ	PHE	1747	16.985	-4.807	4.840	1.00	19.30
ATOM	2529	C	PHE	1747	16.034	-11.049	3.311	1.00	23.57
ATOM	2530	O	PHE	1747	16.182	-11.702	4.344	1.00	25.32
ATOM	2531	N	LYS	1748	15.520	-11.573	2.202	1.00	23.19
ATOM	2533	CA	LYS	1748	15.066	-12.958	2.167	1.00	23.67
ATOM	2534	CB	LYS	1748	14.462	-13.285	0.799	1.00	26.67
ATOM	2535	CG	LYS	1748	14.018	-14.739	0.622	1.00	30.49
ATOM	2536	CD	LYS	1748	13.642	-14.996	-0.837	1.00	38.98
ATOM	2537	CE	LYS	1748	13.182	-16.432	-1.087	1.00	44.52
ATOM	2538	NZ	LYS	1748	11.997	-16.790	-0.245	1.00	52.75
ATOM	2542	C	LYS	1748	16.264	-13.865	2.445	1.00	25.65
ATOM	2543	O	LYS	1748	16.184	-14.778	3.270	1.00	27.19
ATOM	2544	N	GLN	1749	17.378	-13.603	1.762	1.00	24.56
ATOM	2546	CA	GLN	1749	18.588	-14.397	1.950	1.00	26.33
ATOM	2547	CB	GLN	1749	19.702	-13.953	0.993	1.00	27.97
ATOM	2548	CG	GLN	1749	19.416	-14.066	-0.484	1.00	37.31
ATOM	2549	CD	GLN	1749	20.518	-13.415	-1.315	1.00	40.24
ATOM	2550	OE1	GLN	1749	20.296	-12.408	-1.970	1.00	38.83
ATOM	2551	NE2	GLN	1749	21.726	-13.983	-1.259	1.00	47.83
ATOM	2554	C	GLN	1749	19.099	-14.223	3.377	1.00	23.92
ATOM	2555	O	GLN	1749	19.459	-15.196	4.040	1.00	25.27
ATOM	2556	N	LEU	1750	19.155	-12.976	3.829	1.00	23.12
ATOM	2558	CA	LEU	1750	19.641	-12.662	5.175	1.00	24.34
ATOM	2559	CB	LEU	1750	19.607	-11.149	5.427	1.00	23.08
ATOM	2560	CG	LEU	1750	20.633	-10.311	4.665	1.00	23.84
ATOM	2561	CD1	LEU	1750	20.274	-8.806	4.724	1.00	22.10
ATOM	2562	CD2	LEU	1750	22.013	-10.586	5.246	1.00	24.91
ATOM	2563	C	LEU	1750	18.840	-13.400	6.236	1.00	27.40
ATOM	2564	O	LEU	1750	19.408	-13.915	7.211	1.00	27.11
ATOM	2565	N	VAL	1751	17.527	-13.482	6.031	1.00	26.83
ATOM	2567	CA	VAL	1751	16.665	-14.174	6.970	1.00	25.31

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ATOM	2568	CB	VAL	1751	15.176	-13.994	6.599	1.00	25.87
ATOM	2569	CG1	VAL	1751	14.304	-14.975	7.382	1.00	28.43
ATOM	2570	CG2	VAL	1751	14.746	-12.593	6.934	1.00	21.52
ATOM	2571	C	VAL	1751	17.047	-15.642	7.025	1.00	25.87
ATOM	2572	O	VAL	1751	17.178	-16.218	8.106	1.00	23.41
ATOM	2573	N	GLU	1752	17.253	-16.243	5.858	1.00	29.98
ATOM	2575	CA	GLU	1752	17.631	-17.651	5.799	1.00	33.12
ATOM	2576	CB	GLU	1752	17.653	-18.134	4.346	1.00	35.99
ATOM	2577	CG	GLU	1752	16.284	-18.077	3.670	1.00	43.58
ATOM	2578	CD	GLU	1752	16.300	-18.575	2.230	1.00	48.64
ATOM	2579	OE1	GLU	1752	15.453	-18.124	1.431	1.00	48.99
ATOM	2580	OE2	GLU	1752	17.157	-19.426	1.902	1.00	55.41
ATOM	2581	C	GLU	1752	18.995	-17.891	6.467	1.00	33.15
ATOM	2582	O	GLU	1752	19.173	-18.847	7.236	1.00	30.71
ATOM	2583	N	ASP	1753	19.951	-17.011	6.186	1.00	31.12
ATOM	2585	CA	ASP	1753	21.279	-17.131	6.770	1.00	30.51
ATOM	2586	CB	ASP	1753	22.243	-16.108	6.155	1.00	29.15
ATOM	2587	CG	ASP	1753	22.488	-16.344	4.672	1.00	33.53
ATOM	2588	OD1	ASP	1753	22.361	-17.494	4.215	1.00	34.92
ATOM	2589	OD2	ASP	1753	22.815	-15.371	3.955	1.00	38.26
ATOM	2590	C	ASP	1753	21.215	-16.968	8.287	1.00	28.54
ATOM	2591	O	ASP	1753	21.739	-17.800	9.025	1.00	28.95
ATOM	2592	N	LEU	1754	20.537	-15.926	8.753	1.00	27.25
ATOM	2594	CA	LEU	1754	20.421	-15.673	10.193	1.00	28.08
ATOM	2595	CB	LEU	1754	19.754	-14.328	10.455	1.00	23.31
ATOM	2596	CG	LEU	1754	20.733	-13.199	10.160	1.00	24.47
ATOM	2597	CD1	LEU	1754	20.007	-11.863	10.094	1.00	19.58
ATOM	2598	CD2	LEU	1754	21.846	-13.207	11.216	1.00	21.17
ATOM	2599	C	LEU	1754	19.688	-16.789	10.921	1.00	31.61
ATOM	2600	O	LEU	1754	20.037	-17.135	12.048	1.00	32.64
ATOM	2601	N	ASP	1755	18.690	-17.367	10.259	1.00	32.61
ATOM	2603	CA	ASP	1755	17.931	-18.460	10.833	1.00	34.20
ATOM	2604	CB	ASP	1755	16.823	-18.883	9.872	1.00	37.70
ATOM	2605	CG	ASP	1755	15.808	-19.780	10.526	1.00	44.27
ATOM	2606	OD1	ASP	1755	15.445	-19.521	11.692	1.00	47.16
ATOM	2607	OD2	ASP	1755	15.370	-20.745	9.876	1.00	51.35
ATOM	2608	C	ASP	1755	18.894	-19.616	11.073	1.00	34.63
ATOM	2609	O	ASP	1755	18.858	-20.273	12.119	1.00	36.24
ATOM	2610	N	ARG	1756	19.782	-19.826	10.108	1.00	32.60
ATOM	2612	CA	ARG	1756	20.784	-20.870	10.190	1.00	33.69
ATOM	2613	CB	ARG	1756	21.548	-20.939	8.867	1.00	35.42
ATOM	2614	CG	ARG	1756	22.639	-22.003	8.800	1.00	40.87
ATOM	2615	CD	ARG	1756	23.212	-22.094	7.395	1.00	42.73
ATOM	2616	NE	ARG	1756	23.739	-20.813	6.926	1.00	48.45
ATOM	2618	CZ	ARG	1756	24.882	-20.274	7.340	1.00	49.90
ATOM	2619	NH1	ARG	1756	25.634	-20.905	8.243	1.00	49.63
ATOM	2622	NH2	ARG	1756	25.276	-19.105	6.844	1.00	50.86
ATOM	2625	C	ARG	1756	21.748	-20.598	11.345	1.00	34.78
ATOM	2626	O	ARG	1756	21.929	-21.436	12.228	1.00	36.24
ATOM	2627	N	ILE	1757	22.325	-19.402	11.363	1.00	35.35
ATOM	2629	CA	ILE	1757	23.281	-19.018	12.392	1.00	35.54
ATOM	2630	CB	ILE	1757	23.905	-17.631	12.103	1.00	34.99
ATOM	2631	CG2	ILE	1757	24.955	-17.303	13.159	1.00	32.06
ATOM	2632	CG1	ILE	1757	24.547	-17.626	10.711	1.00	33.77

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ATOM	2633	CD1	ILE	1757	24.908	-16.247	10.185	1.00	31.44
ATOM	2634	C	ILE	1757	22.698	-19.036	13.803	1.00	36.49
ATOM	2635	O	ILE	1757	23.337	-19.548	14.716	1.00	36.40
ATOM	2636	N	VAL	1758	21.487	-18.515	13.988	1.00	36.91
ATOM	2638	CA	VAL	1758	20.881	-18.498	15.322	1.00	38.68
ATOM	2639	CB	VAL	1758	19.425	-17.962	15.312	1.00	37.77
ATOM	2640	CG1	VAL	1758	18.806	-18.059	16.708	1.00	38.39
ATOM	2641	CG2	VAL	1758	19.392	-16.524	14.854	1.00	36.69
ATOM	2642	C	VAL	1758	20.891	-19.908	15.895	1.00	41.38
ATOM	2643	O	VAL	1758	21.405	-20.138	16.997	1.00	42.41
ATOM	2644	N	ALA	1759	20.379	-20.851	15.111	1.00	40.59
ATOM	2646	CA	ALA	1759	20.325	-22.247	15.508	1.00	40.84
ATOM	2647	CB	ALA	1759	19.741	-23.074	14.384	1.00	40.20
ATOM	2648	C	ALA	1759	21.703	-22.787	15.897	1.00	42.52
ATOM	2649	O	ALA	1759	21.822	-23.594	16.809	1.00	44.78
ATOM	2650	N	LEU	1760	22.740	-22.339	15.208	1.00	43.16
ATOM	2652	CA	LEU	1760	24.095	-22.800	15.493	1.00	46.98
ATOM	2653	CB	LEU	1760	24.921	-22.761	14.203	1.00	47.66
ATOM	2654	CG	LEU	1760	24.286	-23.545	13.060	1.00	52.77
ATOM	2655	CD1	LEU	1760	24.973	-23.222	11.745	1.00	56.58
ATOM	2656	CD2	LEU	1760	24.343	-25.038	13.369	1.00	53.06
ATOM	2657	C	LEU	1760	24.811	-21.986	16.573	1.00	47.43
ATOM	2658	O	LEU	1760	25.917	-22.335	16.989	1.00	46.58
ATOM	2659	N	THR	1761	24.183	-20.914	17.034	1.00	48.65
ATOM	2661	CA	THR	1761	24.814	-20.055	18.021	1.00	49.69
ATOM	2662	CB	THR	1761	24.382	-18.570	17.831	1.00	50.15
ATOM	2663	OG1	THR	1761	24.783	-18.127	16.529	1.00	49.87
ATOM	2665	CG2	THR	1761	25.063	-17.671	18.843	1.00	48.64
ATOM	2666	C	THR	1761	24.673	-20.497	19.475	1.00	50.33
ATOM	2667	O	THR	1761	23.584	-20.825	19.947	1.00	48.81
ATOM	2668	N	SER	1762	25.811	-20.511	20.166	1.00	50.25
ATOM	2670	CA	SER	1762	25.891	-20.890	21.566	1.00	50.98
ATOM	2671	CB	SER	1762	27.362	-20.887	22.002	1.00	54.71
ATOM	2672	OG	SER	1762	27.537	-21.423	23.308	1.00	57.99
ATOM	2674	C	SER	1762	25.083	-19.914	22.425	1.00	49.39
ATOM	2675	O	SER	1762	25.297	-18.694	22.370	1.00	48.00
ATOM	3474	N	SER	461	79.623	25.766	14.533	1.00	48.84
ATOM	3476	CA	SER	461	79.566	24.645	13.593	1.00	46.93
ATOM	3477	CB	SER	461	78.276	23.838	13.809	1.00	46.66
ATOM	3478	C	SER	461	79.676	25.114	12.138	1.00	43.02
ATOM	3479	O	SER	461	79.692	24.301	11.210	1.00	40.19
ATOM	3480	N	GLU	462	79.791	26.427	11.956	1.00	41.48
ATOM	3482	CA	GLU	462	79.904	27.034	10.628	1.00	39.59
ATOM	3483	CB	GLU	462	80.021	28.560	10.744	1.00	40.66
ATOM	3484	C	GLU	462	81.054	26.480	9.796	1.00	36.60
ATOM	3485	O	GLU	462	80.852	26.121	8.641	1.00	35.10
ATOM	3486	N	TYR	463	82.252	26.416	10.380	1.00	36.07
ATOM	3488	CA	TYR	463	83.430	25.916	9.673	1.00	35.60
ATOM	3489	CB	TYR	463	84.597	26.906	9.755	1.00	38.15
ATOM	3490	CG	TYR	463	84.372	28.104	8.861	1.00	44.08
ATOM	3491	CD1	TYR	463	84.137	29.368	9.406	1.00	44.99
ATOM	3492	CE1	TYR	463	83.833	30.451	8.593	1.00	46.88
ATOM	3493	CD2	TYR	463	84.305	27.959	7.464	1.00	43.95
ATOM	3494	CE2	TYR	463	84.003	29.044	6.642	1.00	41.86

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ATOM	3495	CZ	TYR	463	83.768	30.282	7.215	1.00	43.89
ATOM	3496	OH	TYR	463	83.468	31.364	6.431	1.00	44.37
ATOM	3498	C	TYR	463	83.903	24.520	10.014	1.00	33.90
ATOM	3499	O	TYR	463	84.440	23.828	9.147	1.00	33.90
ATOM	3500	N	GLU	464	83.742	24.098	11.260	1.00	32.81
ATOM	3502	CA	GLU	464	84.167	22.753	11.633	1.00	34.64
ATOM	3503	CB	GLU	464	85.663	22.727	11.919	1.00	37.48
ATOM	3504	CG	GLU	464	86.075	23.633	13.049	1.00	45.48
ATOM	3505	CD	GLU	464	87.552	23.987	13.015	1.00	55.80
ATOM	3506	OE1	GLU	464	87.920	24.996	13.659	1.00	61.78
ATOM	3507	OE2	GLU	464	88.344	23.271	12.351	1.00	58.34
ATOM	3508	C	GLU	464	83.426	22.296	12.858	1.00	33.05
ATOM	3509	O	GLU	464	83.083	23.119	13.705	1.00	34.54
ATOM	3510	N	LEU	465	83.147	21.001	12.943	1.00	32.59
ATOM	3512	CA	LEU	465	82.462	20.463	14.114	1.00	33.74
ATOM	3513	CB	LEU	465	81.484	19.341	13.747	1.00	31.20
ATOM	3514	CG	LEU	465	80.510	19.433	12.577	1.00	32.77
ATOM	3515	CD1	LEU	465	79.355	18.492	12.858	1.00	26.22
ATOM	3516	CD2	LEU	465	80.021	20.846	12.359	1.00	31.59
ATOM	3517	C	LEU	465	83.511	19.889	15.059	1.00	35.64
ATOM	3518	O	LEU	465	84.641	19.574	14.642	1.00	33.77
ATOM	3519	N	PRO	466	83.150	19.734	16.349	1.00	36.71
ATOM	3520	CD	PRO	466	81.865	20.104	16.967	1.00	36.97
ATOM	3521	CA	PRO	466	84.074	19.185	17.346	1.00	36.17
ATOM	3522	CB	PRO	466	83.247	19.196	18.626	1.00	36.83
ATOM	3523	CG	PRO	466	82.274	20.326	18.394	1.00	40.80
ATOM	3524	C	PRO	466	84.419	17.765	16.950	1.00	37.39
ATOM	3525	O	PRO	466	83.626	17.077	16.297	1.00	34.71
ATOM	3526	N	GLU	467	85.611	17.330	17.315	1.00	38.40
ATOM	3528	CA	GLU	467	86.030	15.987	16.976	1.00	42.59
ATOM	3529	CB	GLU	467	87.493	15.987	16.540	1.00	49.21
ATOM	3530	CG	GLU	467	87.922	14.682	15.891	1.00	58.93
ATOM	3531	CD	GLU	467	89.276	14.769	15.213	1.00	64.76
ATOM	3532	OE1	GLU	467	90.013	15.767	15.426	1.00	63.57
ATOM	3533	OE2	GLU	467	89.592	13.823	14.458	1.00	69.03
ATOM	3534	C	GLU	467	85.825	15.037	18.146	1.00	40.74
ATOM	3535	O	GLU	467	85.938	15.430	19.309	1.00	41.52
ATOM	3536	N	ASP	468	85.472	13.802	17.831	1.00	38.57
ATOM	3538	CA	ASP	468	85.273	12.776	18.851	1.00	40.86
ATOM	3539	CB	ASP	468	83.793	12.640	19.224	1.00	40.27
ATOM	3540	CG	ASP	468	83.566	11.697	20.397	1.00	41.36
ATOM	3541	OD1	ASP	468	82.429	11.670	20.919	1.00	42.50
ATOM	3542	OD2	ASP	468	84.514	10.992	20.807	1.00	38.55
ATOM	3543	C	ASP	468	85.803	11.470	18.278	1.00	40.75
ATOM	3544	O	ASP	468	85.068	10.701	17.650	1.00	41.80
ATOM	3545	N	PRO	469	87.100	11.209	18.481	1.00	41.71
ATOM	3546	CD	PRO	469	88.001	12.062	19.276	1.00	41.87
ATOM	3547	CA	PRO	469	87.801	10.011	18.012	1.00	40.07
ATOM	3548	CB	PRO	469	89.091	10.042	18.831	1.00	40.42
ATOM	3549	CG	PRO	469	89.366	11.505	18.938	1.00	39.42
ATOM	3550	C	PRO	469	87.033	8.720	18.260	1.00	41.00
ATOM	3551	O	PRO	469	87.032	7.822	17.414	1.00	41.75
ATOM	3552	N	ARG	470	86.361	8.639	19.411	1.00	40.70
ATOM	3554	CA	ARG	470	85.600	7.446	19.779	1.00	41.03

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ATOM	3555	CB	ARG	470	84.827	7.677	21.075	1.00	44.18
ATOM	3556	CG	ARG	470	85.628	8.240	22.218	1.00	47.89
ATOM	3557	CD	ARG	470	84.719	8.518	23.400	1.00	50.56
ATOM	3558	NE	ARG	470	83.576	9.345	23.023	1.00	51.20
ATOM	3560	CZ	ARG	470	82.695	9.845	23.881	1.00	52.24
ATOM	3561	NH1	ARG	470	82.818	9.608	25.183	1.00	51.31
ATOM	3564	NH2	ARG	470	81.672	10.564	23.432	1.00	52.73
ATOM	3567	C	ARG	470	84.596	7.004	18.723	1.00	39.03
ATOM	3568	O	ARG	470	84.401	5.813	18.518	1.00	40.72
ATOM	3569	N	TRP	471	83.972	7.965	18.050	1.00	37.77
ATOM	3571	CA	TRP	471	82.948	7.656	17.059	1.00	36.73
ATOM	3572	CB	TRP	471	81.672	8.401	17.432	1.00	35.05
ATOM	3573	CG	TRP	471	81.044	7.862	18.673	1.00	34.85
ATOM	3574	CD2	TRP	471	80.235	6.687	18.766	1.00	34.96
ATOM	3575	CE2	TRP	471	79.831	6.564	20.116	1.00	35.12
ATOM	3576	CE3	TRP	471	79.810	5.721	17.838	1.00	33.25
ATOM	3577	CD1	TRP	471	81.106	8.390	19.933	1.00	29.97
ATOM	3578	NE1	TRP	471	80.377	7.616	20.805	1.00	32.18
ATOM	3580	CZ2	TRP	471	79.017	5.512	20.560	1.00	33.98
ATOM	3581	CZ3	TRP	471	79.002	4.673	18.282	1.00	33.71
ATOM	3582	CH2	TRP	471	78.618	4.580	19.632	1.00	33.28
ATOM	3583	C	TRP	471	83.275	7.930	15.599	1.00	37.27
ATOM	3584	O	TRP	471	82.580	7.445	14.695	1.00	36.61
ATOM	3585	N	GLU	472	84.341	8.680	15.361	1.00	37.93
ATOM	3587	CA	GLU	472	84.706	9.054	14.004	1.00	37.08
ATOM	3588	CB	GLU	472	85.865	10.049	14.045	1.00	36.30
ATOM	3589	CG	GLU	472	86.026	10.851	12.773	1.00	33.51
ATOM	3590	CD	GLU	472	84.931	11.895	12.580	1.00	33.80
ATOM	3591	OE1	GLU	472	84.385	12.408	13.581	1.00	35.19
ATOM	3592	OE2	GLU	472	84.641	12.226	11.412	1.00	32.51
ATOM	3593	C	GLU	472	85.021	7.923	13.032	1.00	37.88
ATOM	3594	O	GLU	472	85.774	7.000	13.351	1.00	38.20
ATOM	3595	N	LEU	473	84.422	7.992	11.846	1.00	37.55
ATOM	3597	CA	LEU	473	84.678	7.004	10.813	1.00	36.93
ATOM	3598	CB	LEU	473	83.404	6.244	10.443	1.00	37.08
ATOM	3599	CG	LEU	473	83.680	5.086	9.470	1.00	39.14
ATOM	3600	CD1	LEU	473	84.196	3.877	10.250	1.00	38.39
ATOM	3601	CD2	LEU	473	82.433	4.716	8.672	1.00	39.46
ATOM	3602	C	LEU	473	85.207	7.732	9.577	1.00	38.52
ATOM	3603	O	LEU	473	84.660	8.764	9.182	1.00	38.67
ATOM	3604	N	PRO	474	86.334	7.259	9.005	1.00	39.02
ATOM	3605	CD	PRO	474	87.259	6.259	9.571	1.00	38.39
ATOM	3606	CA	PRO	474	86.918	7.877	7.809	1.00	38.24
ATOM	3607	CB	PRO	474	88.188	7.049	7.590	1.00	38.40
ATOM	3608	CG	PRO	474	88.580	6.680	8.979	1.00	35.50
ATOM	3609	C	PRO	474	85.942	7.727	6.642	1.00	37.56
ATOM	3610	O	PRO	474	85.415	6.641	6.400	1.00	37.88
ATOM	3611	N	ARG	475	85.720	8.809	5.907	1.00	37.73
ATOM	3613	CA	ARG	475	84.779	8.790	4.795	1.00	40.01
ATOM	3614	CB	ARG	475	84.655	10.183	4.182	1.00	38.31
ATOM	3615	CG	ARG	475	84.217	11.236	5.198	1.00	35.15
ATOM	3616	CD	ARG	475	84.069	12.631	4.586	1.00	33.92
ATOM	3617	NE	ARG	475	83.718	13.603	5.616	1.00	30.45
ATOM	3619	CZ	ARG	475	82.475	13.880	5.993	1.00	26.48

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ATOM	3620	NH1	ARG	475	81.444	13.284	5.407	1.00	24.80
ATOM	3623	NH2	ARG	475	82.271	14.650	7.056	1.00	25.16
ATOM	3626	C	ARG	475	85.054	7.735	3.728	1.00	42.18
ATOM	3627	O	ARG	475	84.125	7.197	3.128	1.00	41.43
ATOM	3628	N	ASP	476	86.322	7.391	3.535	1.00	45.44
ATOM	3630	CA	ASP	476	86.676	6.387	2.541	1.00	49.80
ATOM	3631	CB	ASP	476	88.192	6.343	2.329	1.00	50.95
ATOM	3632	CG	ASP	476	88.944	5.975	3.585	1.00	53.89
ATOM	3633	OD1	ASP	476	89.303	4.789	3.731	1.00	59.71
ATOM	3634	OD2	ASP	476	89.176	6.867	4.427	1.00	57.39
ATOM	3635	C	ASP	476	86.149	5.010	2.950	1.00	51.23
ATOM	3636	O	ASP	476	86.051	4.102	2.121	1.00	53.54
ATOM	3637	N	ARG	477	85.814	4.864	4.230	1.00	50.49
ATOM	3639	CA	ARG	477	85.285	3.610	4.753	1.00	49.32
ATOM	3640	CB	ARG	477	85.834	3.364	6.152	1.00	49.79
ATOM	3641	CG	ARG	477	87.237	2.806	6.112	1.00	53.06
ATOM	3642	CD	ARG	477	87.960	2.981	7.420	1.00	56.76
ATOM	3643	NE	ARG	477	87.310	2.293	8.529	1.00	59.35
ATOM	3645	CZ	ARG	477	87.728	2.371	9.789	1.00	62.23
ATOM	3646	NH1	ARG	477	88.793	3.103	10.101	1.00	63.66
ATOM	3649	NH2	ARG	477	87.067	1.741	10.745	1.00	64.35
ATOM	3652	C	ARG	477	83.755	3.547	4.750	1.00	48.04
ATOM	3653	O	ARG	477	83.160	2.693	5.404	1.00	48.09
ATOM	3654	N	LEU	478	83.129	4.412	3.958	1.00	45.38
ATOM	3656	CA	LEU	478	81.685	4.469	3.870	1.00	41.60
ATOM	3657	CB	LEU	478	81.168	5.578	4.790	1.00	38.39
ATOM	3658	CG	LEU	478	79.651	5.699	4.894	1.00	36.38
ATOM	3659	CD1	LEU	478	79.113	4.595	5.802	1.00	33.98
ATOM	3660	CD2	LEU	478	79.293	7.068	5.441	1.00	40.06
ATOM	3661	C	LEU	478	81.279	4.774	2.433	1.00	41.92
ATOM	3662	O	LEU	478	81.696	5.780	1.870	1.00	43.99
ATOM	3663	N	VAL	479	80.466	3.904	1.844	1.00	42.29
ATOM	3665	CA	VAL	479	79.992	4.082	0.471	1.00	41.07
ATOM	3666	CB	VAL	479	80.227	2.816	-0.397	1.00	41.13
ATOM	3667	CG1	VAL	479	79.719	3.057	-1.810	1.00	40.19
ATOM	3668	CG2	VAL	479	81.700	2.448	-0.420	1.00	41.36
ATOM	3669	C	VAL	479	78.500	4.345	0.540	1.00	40.44
ATOM	3670	O	VAL	479	77.719	3.451	0.885	1.00	39.86
ATOM	3671	N	LEU	480	78.112	5.582	0.253	1.00	41.37
ATOM	3673	CA	LEU	480	76.706	5.973	0.293	1.00	41.63
ATOM	3674	CB	LEU	480	76.568	7.492	0.166	1.00	39.91
ATOM	3675	CG	LEU	480	77.236	8.332	1.261	1.00	39.23
ATOM	3676	CD1	LEU	480	76.890	9.800	1.039	1.00	37.73
ATOM	3677	CD2	LEU	480	76.791	7.877	2.647	1.00	35.18
ATOM	3678	C	LEU	480	75.899	5.273	-0.788	1.00	42.21
ATOM	3679	O	LEU	480	76.395	5.048	-1.890	1.00	45.27
ATOM	3680	N	GLY	481	74.650	4.947	-0.476	1.00	41.51
ATOM	3682	CA	GLY	481	73.812	4.257	-1.433	1.00	40.19
ATOM	3683	C	GLY	481	72.446	4.872	-1.640	1.00	41.58
ATOM	3684	O	GLY	481	72.262	6.091	-1.550	1.00	41.35
ATOM	3685	N	LYS	482	71.474	4.009	-1.908	1.00	42.65
ATOM	3687	CA	LYS	482	70.105	4.429	-2.166	1.00	44.17
ATOM	3688	CB	LYS	482	69.240	3.221	-2.542	1.00	45.66
ATOM	3689	C	LYS	482	69.475	5.148	-0.994	1.00	44.86

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ATOM	3690	O	LYS	482	69.638	4.752	0.155	1.00	45.23
ATOM	3691	N	PRO	483	68.749	6.234	-1.273	1.00	45.94
ATOM	3692	CD	PRO	483	68.518	6.880	-2.576	1.00	46.96
ATOM	3693	CA	PRO	483	68.099	6.983	-0.206	1.00	47.79
ATOM	3694	CB	PRO	483	67.542	8.200	-0.947	1.00	47.02
ATOM	3695	CG	PRO	483	67.269	7.666	-2.307	1.00	46.65
ATOM	3696	C	PRO	483	66.991	6.151	0.429	1.00	48.74
ATOM	3697	O	PRO	483	66.314	5.376	-0.251	1.00	48.01
ATOM	3698	N	LEU	484	66.858	6.268	1.742	1.00	49.91
ATOM	3700	CA	LEU	484	65.837	5.547	2.477	1.00	53.93
ATOM	3701	CB	LEU	484	66.433	4.883	3.720	1.00	50.17
ATOM	3702	CG	LEU	484	67.517	3.844	3.445	1.00	48.93
ATOM	3703	CD1	LEU	484	68.226	3.460	4.731	1.00	49.05
ATOM	3704	CD2	LEU	484	66.906	2.630	2.784	1.00	47.03
ATOM	3705	C	LEU	484	64.715	6.501	2.878	1.00	58.70
ATOM	3706	O	LEU	484	63.571	6.075	3.055	1.00	61.95
ATOM	3707	N	GLY	485	65.027	7.788	3.006	1.00	60.35
ATOM	3709	CA	GLY	485	63.998	8.737	3.397	1.00	64.00
ATOM	3710	C	GLY	485	64.445	10.183	3.476	1.00	66.09
ATOM	3711	O	GLY	485	65.643	10.468	3.577	1.00	65.26
ATOM	3712	N	GLU	486	63.471	11.090	3.458	1.00	67.18
ATOM	3714	CA	GLU	486	63.733	12.525	3.508	1.00	68.69
ATOM	3715	CB	GLU	486	63.873	13.084	2.091	1.00	69.88
ATOM	3716	C	GLU	486	62.618	13.249	4.245	1.00	68.80
ATOM	3717	O	GLU	486	61.481	12.775	4.295	1.00	69.26
ATOM	3718	N	GLY	487	62.943	14.415	4.791	1.00	68.47
ATOM	3720	CA	GLY	487	61.960	15.188	5.520	1.00	67.56
ATOM	3721	C	GLY	487	62.373	16.635	5.634	1.00	66.71
ATOM	3722	O	GLY	487	63.040	17.172	4.747	1.00	66.48
ATOM	3723	N	ALA	488	61.979	17.265	6.735	1.00	67.22
ATOM	3725	CA	ALA	488	62.304	18.661	6.992	1.00	67.78
ATOM	3726	CB	ALA	488	61.637	19.121	8.283	1.00	68.97
ATOM	3727	C	ALA	488	63.817	18.830	7.085	1.00	67.38
ATOM	3728	O	ALA	488	64.413	18.597	8.141	1.00	67.14
ATOM	3729	N	PHE	489	64.429	19.155	5.946	1.00	66.22
ATOM	3731	CA	PHE	489	65.877	19.364	5.831	1.00	65.49
ATOM	3732	CB	PHE	489	66.277	20.699	6.467	1.00	66.11
ATOM	3733	C	PHE	489	66.749	18.207	6.368	1.00	64.07
ATOM	3734	O	PHE	489	67.924	18.399	6.731	1.00	61.56
ATOM	3735	N	GLY	490	66.171	17.005	6.349	1.00	60.79
ATOM	3737	CA	GLY	490	66.852	15.803	6.797	1.00	54.72
ATOM	3738	C	GLY	490	66.787	14.760	5.692	1.00	51.78
ATOM	3739	O	GLY	490	65.765	14.624	5.013	1.00	49.17
ATOM	3740	N	GLN	491	67.874	14.015	5.528	1.00	49.97
ATOM	3742	CA	GLN	491	68.000	12.984	4.504	1.00	48.06
ATOM	3743	CB	GLN	491	68.891	13.520	3.371	1.00	51.02
ATOM	3744	CG	GLN	491	69.286	12.518	2.289	1.00	56.00
ATOM	3745	CD	GLN	491	70.155	13.143	1.202	1.00	58.93
ATOM	3746	OE1	GLN	491	70.483	14.330	1.255	1.00	60.31
ATOM	3747	NE2	GLN	491	70.529	12.341	0.202	1.00	60.19
ATOM	3750	C	GLN	491	68.623	11.720	5.114	1.00	45.59
ATOM	3751	O	GLN	491	69.511	11.792	5.959	1.00	45.22
ATOM	3752	N	VAL	492	68.148	10.561	4.693	1.00	43.19
ATOM	3754	CA	VAL	492	68.676	9.304	5.193	1.00	41.54

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ATOM	3755	CB	VAL	492	67.655	8.584	6.087	1.00	41.74
ATOM	3756	CG1	VAL	492	68.217	7.248	6.561	1.00	43.70
ATOM	3757	CG2	VAL	492	67.283	9.463	7.269	1.00	44.07
ATOM	3758	C	VAL	492	68.971	8.424	3.993	1.00	39.72
ATOM	3759	O	VAL	492	68.125	8.271	3.108	1.00	39.81
ATOM	3760	N	VAL	493	70.176	7.872	3.942	1.00	36.38
ATOM	3762	CA	VAL	493	70.545	7.001	2.844	1.00	35.88
ATOM	3763	CB	VAL	493	71.580	7.666	1.869	1.00	36.92
ATOM	3764	CG1	VAL	493	71.142	9.069	1.485	1.00	36.64
ATOM	3765	CG2	VAL	493	72.978	7.670	2.469	1.00	38.29
ATOM	3766	C	VAL	493	71.131	5.689	3.351	1.00	36.03
ATOM	3767	O	VAL	493	71.693	5.617	4.443	1.00	36.57
ATOM	3768	N	LEU	494	70.947	4.637	2.571	1.00	34.91
ATOM	3770	CA	LEU	494	71.500	3.344	2.909	1.00	36.04
ATOM	3771	CB	LEU	494	70.809	2.244	2.094	1.00	37.43
ATOM	3772	CG	LEU	494	71.312	0.814	2.269	1.00	36.62
ATOM	3773	CD1	LEU	494	71.327	0.437	3.735	1.00	36.37
ATOM	3774	CD2	LEU	494	70.419	-0.118	1.479	1.00	40.70
ATOM	3775	C	LEU	494	72.967	3.451	2.510	1.00	37.08
ATOM	3776	O	LEU	494	73.308	4.160	1.560	1.00	34.90
ATOM	3777	N	ALA	495	73.839	2.779	3.243	1.00	37.18
ATOM	3779	CA	ALA	495	75.246	2.830	2.918	1.00	39.84
ATOM	3780	CB	ALA	495	75.885	4.066	3.541	1.00	39.29
ATOM	3781	C	ALA	495	75.949	1.578	3.400	1.00	41.68
ATOM	3782	O	ALA	495	75.400	0.808	4.189	1.00	41.53
ATOM	3783	N	GLU	496	77.149	1.348	2.881	1.00	43.44
ATOM	3785	CA	GLU	496	77.936	0.202	3.297	1.00	42.86
ATOM	3786	CB	GLU	496	78.328	-0.663	2.101	1.00	44.63
ATOM	3787	CG	GLU	496	77.120	-1.167	1.320	1.00	53.31
ATOM	3788	CD	GLU	496	77.386	-2.450	0.545	1.00	59.48
ATOM	3789	OE1	GLU	496	76.494	-3.332	0.534	1.00	62.39
ATOM	3790	OE2	GLU	496	78.477	-2.580	-0.053	1.00	62.15
ATOM	3791	C	GLU	496	79.150	0.750	4.006	1.00	40.96
ATOM	3792	O	GLU	496	79.889	1.568	3.455	1.00	40.81
ATOM	3793	N	ALA	497	79.267	0.411	5.280	1.00	40.79
ATOM	3795	CA	ALA	497	80.381	0.857	6.096	1.00	41.84
ATOM	3796	CB	ALA	497	79.888	1.240	7.478	1.00	38.80
ATOM	3797	C	ALA	497	81.394	-0.280	6.181	1.00	44.72
ATOM	3798	O	ALA	497	81.019	-1.445	6.215	1.00	44.78
ATOM	3799	N	ILE	498	82.678	0.054	6.183	1.00	48.03
ATOM	3801	CA	ILE	498	83.729	-0.952	6.255	1.00	48.78
ATOM	3802	CB	ILE	498	84.654	-0.894	5.014	1.00	50.57
ATOM	3803	CG2	ILE	498	85.748	-1.954	5.119	1.00	51.32
ATOM	3804	CG1	ILE	498	83.851	-1.103	3.726	1.00	51.90
ATOM	3805	CD1	ILE	498	83.139	0.146	3.198	1.00	55.47
ATOM	3806	C	ILE	498	84.573	-0.754	7.511	1.00	48.31
ATOM	3807	O	ILE	498	85.005	0.359	7.805	1.00	47.90
ATOM	3808	N	GLY	499	84.754	-1.829	8.271	1.00	49.29
ATOM	3810	CA	GLY	499	85.563	-1.774	9.479	1.00	53.17
ATOM	3811	C	GLY	499	85.076	-0.944	10.657	1.00	57.22
ATOM	3812	O	GLY	499	85.885	-0.341	11.364	1.00	59.20
ATOM	3813	N	LEU	500	83.768	-0.948	10.909	1.00	58.51
ATOM	3815	CA	LEU	500	83.193	-0.189	12.025	1.00	57.80
ATOM	3816	CB	LEU	500	81.705	-0.519	12.181	1.00	55.67

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ATOM	3817	CG	LEU	500	80.789	0.036	11.086	1.00	54.81
ATOM	3818	CD1	LEU	500	79.361	-0.445	11.293	1.00	53.00
ATOM	3819	CD2	LEU	500	80.854	1.561	11.089	1.00	53.27
ATOM	3820	C	LEU	500	83.926	-0.466	13.333	1.00	58.15
ATOM	3821	O	LEU	500	84.461	-1.560	13.529	1.00	60.29
ATOM	3822	N	PRO	505	87.397	-6.022	10.511	1.00	77.18
ATOM	3823	CD	PRO	505	88.509	-6.651	11.242	1.00	78.26
ATOM	3824	CA	PRO	505	87.755	-4.660	10.097	1.00	75.62
ATOM	3825	CB	PRO	505	89.166	-4.487	10.669	1.00	75.77
ATOM	3826	CG	PRO	505	89.696	-5.884	10.715	1.00	77.07
ATOM	3827	C	PRO	505	87.709	-4.440	8.583	1.00	73.15
ATOM	3828	O	PRO	505	87.772	-3.308	8.105	1.00	72.63
ATOM	3829	N	ASN	506	87.595	-5.524	7.830	1.00	71.27
ATOM	3831	CA	ASN	506	87.518	-5.421	6.380	1.00	69.14
ATOM	3832	CB	ASN	506	88.577	-6.313	5.728	1.00	70.76
ATOM	3833	C	ASN	506	86.119	-5.840	5.940	1.00	67.30
ATOM	3834	O	ASN	506	85.834	-5.957	4.750	1.00	67.03
ATOM	3835	N	ARG	507	85.250	-6.064	6.921	1.00	65.27
ATOM	3837	CA	ARG	507	83.876	-6.479	6.669	1.00	62.86
ATOM	3838	CB	ARG	507	83.335	-7.267	7.864	1.00	65.45
ATOM	3839	C	ARG	507	82.991	-5.274	6.443	1.00	59.56
ATOM	3840	O	ARG	507	83.161	-4.247	7.100	1.00	59.70
ATOM	3841	N	VAL	508	82.057	-5.397	5.509	1.00	56.65
ATOM	3843	CA	VAL	508	81.135	-4.310	5.226	1.00	55.48
ATOM	3844	CB	VAL	508	80.850	-4.157	3.719	1.00	55.71
ATOM	3845	CG1	VAL	508	82.146	-3.962	2.962	1.00	58.18
ATOM	3846	CG2	VAL	508	80.096	-5.356	3.188	1.00	58.76
ATOM	3847	C	VAL	508	79.833	-4.537	5.979	1.00	53.10
ATOM	3848	O	VAL	508	79.352	-5.665	6.091	1.00	54.25
ATOM	3849	N	THR	509	79.282	-3.460	6.514	1.00	50.06
ATOM	3851	CA	THR	509	78.041	-3.512	7.260	1.00	45.70
ATOM	3852	CB	THR	509	78.256	-3.029	8.715	1.00	45.59
ATOM	3853	OG1	THR	509	79.395	-3.696	9.279	1.00	43.86
ATOM	3855	CG2	THR	509	77.028	-3.328	9.573	1.00	44.19
ATOM	3856	C	THR	509	77.064	-2.574	6.564	1.00	43.57
ATOM	3857	O	THR	509	77.416	-1.444	6.221	1.00	41.15
ATOM	3858	N	LYS	510	75.871	-3.073	6.268	1.00	42.96
ATOM	3860	CA	LYS	510	74.847	-2.253	5.640	1.00	41.91
ATOM	3861	CB	LYS	510	73.740	-3.144	5.091	1.00	44.74
ATOM	3862	CG	LYS	510	72.864	-2.461	4.069	1.00	51.83
ATOM	3863	CD	LYS	510	73.392	-2.645	2.659	1.00	55.00
ATOM	3864	CE	LYS	510	72.769	-3.879	2.020	1.00	58.36
ATOM	3865	NZ	LYS	510	73.069	-5.131	2.769	1.00	58.57
ATOM	3869	C	LYS	510	74.322	-1.367	6.789	1.00	40.74
ATOM	3870	O	LYS	510	73.909	-1.874	7.837	1.00	40.26
ATOM	3871	N	VAL	511	74.413	-0.052	6.624	1.00	37.21
ATOM	3873	CA	VAL	511	73.989	0.877	7.661	1.00	33.44
ATOM	3874	CB	VAL	511	75.227	1.515	8.362	1.00	34.53
ATOM	3875	CG1	VAL	511	76.100	0.436	9.014	1.00	31.98
ATOM	3876	CG2	VAL	511	76.048	2.322	7.358	1.00	34.82
ATOM	3877	C	VAL	511	73.134	1.989	7.087	1.00	31.34
ATOM	3878	O	VAL	511	73.025	2.130	5.871	1.00	31.33
ATOM	3879	N	ALA	512	72.485	2.748	7.961	1.00	30.70
ATOM	3881	CA	ALA	512	71.671	3.876	7.523	1.00	30.81

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ATOM	3882	CB	ALA	512	70.305	3.879	8.206	1.00	29.85
ATOM	3883	C	ALA	512	72.453	5.124	7.904	1.00	31.30
ATOM	3884	O	ALA	512	73.036	5.197	8.996	1.00	30.24
ATOM	3885	N	VAL	513	72.480	6.096	6.999	1.00	30.86
ATOM	3887	CA	VAL	513	73.208	7.332	7.238	1.00	30.58
ATOM	3888	CB	VAL	513	74.358	7.525	6.223	1.00	31.11
ATOM	3889	CG1	VAL	513	75.132	8.788	6.547	1.00	29.63
ATOM	3890	CG2	VAL	513	75.290	6.317	6.223	1.00	28.70
ATOM	3891	C	VAL	513	72.300	8.556	7.189	1.00	31.28
ATOM	3892	O	VAL	513	71.645	8.824	6.167	1.00	30.12
ATOM	3893	N	LYS	514	72.229	9.257	8.321	1.00	31.03
ATOM	3895	CA	LYS	514	71.439	10.479	8.451	1.00	32.56
ATOM	3896	CB	LYS	514	70.881	10.635	9.870	1.00	34.31
ATOM	3897	CG	LYS	514	69.977	9.516	10.326	1.00	38.25
ATOM	3898	CD	LYS	514	69.513	9.774	11.753	1.00	47.74
ATOM	3899	CE	LYS	514	68.514	8.719	12.230	1.00	51.60
ATOM	3900	NZ	LYS	514	67.226	8.755	11.468	1.00	58.53
ATOM	3904	C	LYS	514	72.357	11.659	8.137	1.00	30.29
ATOM	3905	O	LYS	514	73.485	11.736	8.628	1.00	28.14
ATOM	3906	N	MET	515	71.867	12.580	7.320	1.00	30.67
ATOM	3908	CA	MET	515	72.643	13.747	6.920	1.00	29.94
ATOM	3909	CB	MET	515	73.435	13.442	5.648	1.00	30.64
ATOM	3910	CG	MET	515	72.557	13.038	4.464	1.00	32.16
ATOM	3911	SD	MET	515	73.525	12.522	3.036	1.00	37.59
ATOM	3912	CE	MET	515	74.015	10.933	3.563	1.00	29.11
ATOM	3913	C	MET	515	71.675	14.869	6.635	1.00	29.71
ATOM	3914	O	MET	515	70.462	14.664	6.598	1.00	30.04
ATOM	3915	N	LEU	516	72.212	16.060	6.445	1.00	29.56
ATOM	3917	CA	LEU	516	71.381	17.206	6.136	1.00	30.76
ATOM	3918	CB	LEU	516	72.093	18.508	6.526	1.00	28.20
ATOM	3919	CG	LEU	516	72.396	18.724	8.011	1.00	28.48
ATOM	3920	CD1	LEU	516	73.202	19.983	8.185	1.00	27.55
ATOM	3921	CD2	LEU	516	71.114	18.814	8.794	1.00	25.49
ATOM	3922	C	LEU	516	71.081	17.225	4.647	1.00	30.97
ATOM	3923	O	LEU	516	71.728	16.534	3.851	1.00	29.93
ATOM	3924	N	LYS	517	70.030	17.946	4.291	1.00	31.57
ATOM	3926	CA	LYS	517	69.677	18.117	2.899	1.00	31.44
ATOM	3927	CB	LYS	517	68.169	18.310	2.752	1.00	34.79
ATOM	3928	CG	LYS	517	67.375	17.098	3.194	1.00	38.42
ATOM	3929	CD	LYS	517	66.148	16.888	2.343	1.00	46.52
ATOM	3930	CE	LYS	517	65.087	17.950	2.582	1.00	53.77
ATOM	3931	NZ	LYS	517	63.901	17.740	1.690	1.00	56.38
ATOM	3935	C	LYS	517	70.457	19.377	2.499	1.00	30.18
ATOM	3936	O	LYS	517	70.892	20.134	3.370	1.00	27.47
ATOM	3937	N	SER	518	70.646	19.594	1.201	1.00	31.13
ATOM	3939	CA	SER	518	71.394	20.747	0.693	1.00	32.11
ATOM	3940	CB	SER	518	71.518	20.652	-0.824	1.00	33.45
ATOM	3941	OG	SER	518	70.242	20.567	-1.428	1.00	34.51
ATOM	3943	C	SER	518	70.814	22.103	1.073	1.00	32.81
ATOM	3944	O	SER	518	71.515	23.123	1.027	1.00	34.03
ATOM	3945	N	ASP	519	69.540	22.117	1.449	1.00	29.80
ATOM	3947	CA	ASP	519	68.886	23.354	1.836	1.00	28.94
ATOM	3948	CB	ASP	519	67.473	23.421	1.237	1.00	33.90
ATOM	3949	CG	ASP	519	66.542	22.332	1.771	1.00	34.42

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ATOM	3950	OD1	ASP	519	67.020	21.328	2.333	1.00	35.58
ATOM	3951	OD2	ASP	519	65.313	22.485	1.617	1.00	41.83
ATOM	3952	C	ASP	519	68.829	23.559	3.342	1.00	29.08
ATOM	3953	O	ASP	519	68.177	24.485	3.816	1.00	29.79
ATOM	3954	N	ALA	520	69.514	22.710	4.099	1.00	29.73
ATOM	3956	CA	ALA	520	69.488	22.824	5.558	1.00	29.16
ATOM	3957	CB	ALA	520	70.174	21.639	6.190	1.00	28.13
ATOM	3958	C	ALA	520	70.122	24.108	6.040	1.00	28.06
ATOM	3959	O	ALA	520	70.880	24.741	5.309	1.00	28.84
ATOM	3960	N	THR	521	69.800	24.491	7.272	1.00	27.84
ATOM	3962	CA	THR	521	70.357	25.692	7.885	1.00	30.45
ATOM	3963	CB	THR	521	69.254	26.635	8.463	1.00	33.56
ATOM	3964	OG1	THR	521	68.547	25.968	9.520	1.00	36.27
ATOM	3966	CG2	THR	521	68.275	27.074	7.379	1.00	36.06
ATOM	3967	C	THR	521	71.251	25.263	9.048	1.00	30.04
ATOM	3968	O	THR	521	71.348	24.072	9.369	1.00	28.16
ATOM	3969	N	GLU	522	71.876	26.241	9.696	1.00	31.42
ATOM	3971	CA	GLU	522	72.745	25.978	10.832	1.00	36.94
ATOM	3972	CB	GLU	522	73.404	27.282	11.299	1.00	44.74
ATOM	3973	CG	GLU	522	74.414	27.130	12.450	1.00	58.34
ATOM	3974	CD	GLU	522	75.769	26.579	12.009	1.00	64.50
ATOM	3975	OE1	GLU	522	76.798	27.261	12.231	1.00	64.89
ATOM	3976	OE2	GLU	522	75.806	25.461	11.452	1.00	70.26
ATOM	3977	C	GLU	522	71.932	25.345	11.969	1.00	34.02
ATOM	3978	O	GLU	522	72.428	24.480	12.684	1.00	31.11
ATOM	3979	N	LYS	523	70.670	25.750	12.097	1.00	32.53
ATOM	3981	CA	LYS	523	69.805	25.210	13.135	1.00	34.06
ATOM	3982	CB	LYS	523	68.481	25.970	13.188	1.00	39.54
ATOM	3983	CG	LYS	523	67.560	25.541	14.322	1.00	45.55
ATOM	3984	CD	LYS	523	66.360	24.776	13.789	1.00	52.08
ATOM	3985	CE	LYS	523	65.443	24.312	14.914	1.00	54.16
ATOM	3986	NZ	LYS	523	64.313	23.509	14.373	1.00	54.38
ATOM	3990	C	LYS	523	69.572	23.733	12.861	1.00	31.73
ATOM	3991	O	LYS	523	69.589	22.922	13.788	1.00	31.15
ATOM	3992	N	ASP	524	69.374	23.383	11.590	1.00	29.22
ATOM	3994	CA	ASP	524	69.182	21.980	11.214	1.00	28.79
ATOM	3995	CB	ASP	524	68.928	21.831	9.714	1.00	27.65
ATOM	3996	CG	ASP	524	67.586	22.396	9.286	1.00	33.89
ATOM	3997	OD1	ASP	524	66.568	22.106	9.954	1.00	34.66
ATOM	3998	OD2	ASP	524	67.549	23.120	8.270	1.00	30.04
ATOM	3999	C	ASP	524	70.424	21.190	11.606	1.00	28.00
ATOM	4000	O	ASP	524	70.317	20.104	12.162	1.00	30.83
ATOM	4001	N	LEU	525	71.603	21.761	11.347	1.00	29.87
ATOM	4003	CA	LEU	525	72.873	21.121	11.700	1.00	27.60
ATOM	4004	CB	LEU	525	74.064	21.997	11.282	1.00	24.08
ATOM	4005	CG	LEU	525	75.462	21.433	11.593	1.00	26.11
ATOM	4006	CD1	LEU	525	75.597	19.979	11.098	1.00	23.67
ATOM	4007	CD2	LEU	525	76.530	22.321	10.967	1.00	21.28
ATOM	4008	C	LEU	525	72.909	20.869	13.200	1.00	26.38
ATOM	4009	O	LEU	525	73.249	19.777	13.653	1.00	26.09
ATOM	4010	N	SER	526	72.560	21.902	13.956	1.00	29.72
ATOM	4012	CA	SER	526	72.500	21.861	15.422	1.00	32.16
ATOM	4013	CB	SER	526	71.980	23.209	15.939	1.00	33.45
ATOM	4014	OG	SER	526	71.793	23.213	17.343	1.00	40.42

ATOM	4016	C	SER	526	71.572	20.728	15.902	1.00	31.64
ATOM	4017	O	SER	526	71.869	20.030	16.889	1.00	32.54
ATOM	4018	N	ASP	527	70.454	20.561	15.201	1.00	27.92
ATOM	4020	CA	ASP	527	69.492	19.527	15.524	1.00	28.60
ATOM	4021	CB	ASP	527	68.187	19.767	14.765	1.00	29.35
ATOM	4022	CG	ASP	527	67.418	20.984	15.278	1.00	31.37
ATOM	4023	OD1	ASP	527	67.759	21.549	16.353	1.00	31.96
ATOM	4024	OD2	ASP	527	66.456	21.369	14.591	1.00	32.58
ATOM	4025	C	ASP	527	70.038	18.131	15.246	1.00	28.82
ATOM	4026	O	ASP	527	69.854	17.212	16.047	1.00	29.65
ATOM	4027	N	LEU	528	70.721	17.962	14.120	1.00	29.29
ATOM	4029	CA	LEU	528	71.302	16.658	13.794	1.00	29.94
ATOM	4030	CB	LEU	528	71.780	16.621	12.336	1.00	26.45
ATOM	4031	CG	LEU	528	72.315	15.276	11.840	1.00	28.34
ATOM	4032	CD1	LEU	528	71.240	14.189	12.035	1.00	27.16
ATOM	4033	CD2	LEU	528	72.756	15.387	10.372	1.00	25.91
ATOM	4034	C	LEU	528	72.449	16.319	14.776	1.00	29.72
ATOM	4035	O	LEU	528	72.617	15.162	15.178	1.00	28.98
ATOM	4036	N	ILE	529	73.224	17.329	15.168	1.00	30.15
ATOM	4038	CA	ILE	529	74.305	17.131	16.134	1.00	28.88
ATOM	4039	CB	ILE	529	75.188	18.382	16.268	1.00	26.91
ATOM	4040	CG2	ILE	529	76.175	18.221	17.423	1.00	24.82
ATOM	4041	CG1	ILE	529	75.960	18.613	14.984	1.00	23.98
ATOM	4042	CD1	ILE	529	76.663	19.932	14.973	1.00	28.33
ATOM	4043	C	ILE	529	73.709	16.799	17.518	1.00	29.71
ATOM	4044	O	ILE	529	74.172	15.880	18.193	1.00	29.19
ATOM	4045	N	SER	530	72.672	17.524	17.926	1.00	26.84
ATOM	4047	CA	SER	530	72.061	17.247	19.214	1.00	31.46
ATOM	4048	CB	SER	530	70.948	18.251	19.521	1.00	36.17
ATOM	4049	OG	SER	530	70.045	18.363	18.431	1.00	47.58
ATOM	4051	C	SER	530	71.526	15.822	19.248	1.00	30.05
ATOM	4052	O	SER	530	71.646	15.136	20.270	1.00	29.61
ATOM	4053	N	GLU	531	70.972	15.357	18.132	1.00	27.74
ATOM	4055	CA	GLU	531	70.458	13.999	18.090	1.00	28.71
ATOM	4056	CB	GLU	531	69.709	13.727	16.789	1.00	29.72
ATOM	4057	CG	GLU	531	69.147	12.319	16.737	1.00	32.21
ATOM	4058	CD	GLU	531	68.510	11.979	15.414	1.00	33.88
ATOM	4059	OE1	GLU	531	68.026	10.846	15.281	1.00	37.60
ATOM	4060	OE2	GLU	531	68.483	12.833	14.510	1.00	34.70
ATOM	4061	C	GLU	531	71.578	12.974	18.271	1.00	28.91
ATOM	4062	O	GLU	531	71.428	12.007	19.019	1.00	29.46
ATOM	4063	N	MET	532	72.686	13.179	17.567	1.00	28.84
ATOM	4065	CA	MET	532	73.851	12.296	17.648	1.00	29.35
ATOM	4066	CB	MET	532	74.948	12.786	16.689	1.00	27.41
ATOM	4067	CG	MET	532	76.299	12.117	16.872	1.00	26.71
ATOM	4068	SD	MET	532	77.503	12.675	15.640	1.00	32.27
ATOM	4069	CE	MET	532	77.732	14.400	16.117	1.00	24.10
ATOM	4070	C	MET	532	74.389	12.280	19.078	1.00	28.80
ATOM	4071	O	MET	532	74.700	11.230	19.630	1.00	29.74
ATOM	4072	N	GLU	533	74.481	13.454	19.681	1.00	28.83
ATOM	4074	CA	GLU	533	74.985	13.546	21.033	1.00	29.66
ATOM	4075	CB	GLU	533	75.182	15.008	21.423	1.00	32.23
ATOM	4076	CG	GLU	533	76.331	15.687	20.651	1.00	34.47
ATOM	4077	CD	GLU	533	77.656	14.937	20.774	1.00	38.03

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ATOM	4078	OE1	GLU	533	78.168	14.780	21.903	1.00	39.75	
ATOM	4079	OE2	GLU	533	78.192	14.497	19.736	1.00	38.75	
ATOM	4080	C	GLU	533	74.058	12.815	22.005	1.00	31.55	
ATOM	4081	O	GLU	533	74.521	12.083	22.889	1.00	30.63	
ATOM	4082	N	MET	534	72.750	12.958	21.799	1.00	31.31	
ATOM	4084	CA	MET	534	71.789	12.289	22.664	1.00	30.78	
ATOM	4085	CB	MET	534	70.348	12.672	22.319	1.00	31.23	
ATOM	4086	CG	MET	534	69.453	12.648	23.551	0.50	29.35	PRT1
ATOM	4087	SD	MET	534	67.688	12.563	23.246	0.50	28.79	PRT1
ATOM	4088	CE	MET	534	67.290	14.230	22.875	0.50	26.96	PRT1
ATOM	4089	C	MET	534	71.991	10.773	22.560	1.00	28.82	
ATOM	4090	O	MET	534	72.053	10.083	23.568	1.00	30.10	
ATOM	4091	N	MET	535	72.149	10.271	21.339	1.00	29.16	
ATOM	4093	CA	MET	535	72.381	8.852	21.110	1.00	29.37	
ATOM	4094	CB	MET	535	72.546	8.551	19.617	1.00	27.35	
ATOM	4095	CG	MET	535	71.281	8.790	18.817	1.00	28.40	
ATOM	4096	SD	MET	535	71.255	7.955	17.255	1.00	30.26	
ATOM	4097	CE	MET	535	71.336	9.279	16.188	1.00	35.50	
ATOM	4098	C	MET	535	73.612	8.388	21.887	1.00	30.36	
ATOM	4099	O	MET	535	73.626	7.287	22.460	1.00	26.13	
ATOM	4100	N	LYS	536	74.640	9.233	21.909	1.00	30.70	
ATOM	4102	CA	LYS	536	75.850	8.913	22.649	1.00	31.76	
ATOM	4103	CB	LYS	536	76.934	9.954	22.388	1.00	31.05	
ATOM	4104	CG	LYS	536	77.550	9.883	21.004	1.00	26.80	
ATOM	4105	CD	LYS	536	78.534	11.017	20.860	1.00	31.05	
ATOM	4106	CE	LYS	536	79.132	11.138	19.466	1.00	29.83	
ATOM	4107	NZ	LYS	536	79.957	12.377	19.440	1.00	29.32	
ATOM	4111	C	LYS	536	75.550	8.834	24.150	1.00	31.99	
ATOM	4112	O	LYS	536	75.920	7.859	24.806	1.00	31.92	
ATOM	4113	N	MET	537	74.837	9.826	24.676	1.00	31.81	
ATOM	4115	CA	MET	537	74.517	9.835	26.090	1.00	35.37	
ATOM	4116	CB	MET	537	73.860	11.154	26.506	1.00	41.32	
ATOM	4117	CG	MET	537	74.828	12.335	26.610	1.00	51.50	
ATOM	4118	SD	MET	537	76.234	12.090	27.776	1.00	57.48	
ATOM	4119	CE	MET	537	75.460	12.637	29.334	1.00	56.91	
ATOM	4120	C	MET	537	73.630	8.679	26.499	1.00	36.11	
ATOM	4121	O	MET	537	73.845	8.084	27.548	1.00	38.54	
ATOM	4122	N	ILE	538	72.652	8.347	25.661	1.00	33.69	
ATOM	4124	CA	ILE	538	71.704	7.277	25.954	1.00	31.62	
ATOM	4125	CB	ILE	538	70.492	7.314	24.974	1.00	28.21	
ATOM	4126	CG2	ILE	538	69.681	6.013	25.034	1.00	28.22	
ATOM	4127	CG1	ILE	538	69.590	8.488	25.338	1.00	23.74	
ATOM	4128	CD1	ILE	538	68.487	8.728	24.344	1.00	27.94	
ATOM	4129	C	ILE	538	72.322	5.894	26.008	1.00	31.07	
ATOM	4130	O	ILE	538	71.952	5.080	26.860	1.00	33.13	
ATOM	4131	N	GLY	539	73.239	5.611	25.094	1.00	29.52	
ATOM	4133	CA	GLY	539	73.871	4.309	25.093	1.00	28.40	
ATOM	4134	C	GLY	539	73.111	3.275	24.289	1.00	30.21	
ATOM	4135	O	GLY	539	72.018	3.554	23.788	1.00	29.66	
ATOM	4136	N	LYS	540	73.679	2.074	24.199	1.00	28.44	
ATOM	4138	CA	LYS	540	73.105	0.984	23.426	1.00	31.09	
ATOM	4139	CB	LYS	540	74.215	0.089	22.895	1.00	33.15	
ATOM	4140	CG	LYS	540	75.116	0.776	21.906	1.00	39.54	
ATOM	4141	CD	LYS	540	76.125	-0.175	21.329	1.00	43.98	

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ATOM	4142	CE	LYS	540	77.033				
ATOM	4143	NZ	LYS	540	76.338	0.562	20.349	1.00	50.79
ATOM	4147	C	LYS	540	72.053	0.977	19.086	1.00	51.09
ATOM	4148	O	LYS	540	72.088	0.087	24.059	1.00	32.78
ATOM	4149	N	HIS	541	71.137	-0.195	25.266	1.00	32.41
ATOM	4151	CA	HIS	541	70.080	-0.374	23.208	1.00	31.20
ATOM	4152	CB	HIS	541	68.911	-1.304	23.591	1.00	31.53
ATOM	4153	CG	HIS	541	67.948	-0.630	24.298	1.00	30.69
ATOM	4154	CD2	HIS	541	67.938	-1.613	24.882	1.00	31.18
ATOM	4155	ND1	HIS	541	66.882	-2.255	26.072	1.00	33.02
ATOM	4157	CE1	HIS	541	66.268	-2.123	24.165	1.00	30.56
ATOM	4158	NE2	HIS	541	66.886	-3.037	24.889	1.00	32.95
ATOM	4160	C	HIS	541	69.590	-3.140	26.053	1.00	31.79
ATOM	4161	O	HIS	541	69.495	-2.013	22.340	1.00	32.72
ATOM	4162	N	LYS	542	69.282	-1.404	21.275	1.00	30.34
ATOM	4164	CA	LYS	542	68.828	-3.305	22.475	1.00	32.32
ATOM	4165	CB	LYS	542	68.637	-4.131	21.359	1.00	30.29
ATOM	4166	C	LYS	542	67.560	-5.587	21.798	1.00	29.34
ATOM	4167	O	LYS	542	67.369	-3.661	20.692	1.00	29.09
ATOM	4168	N	ASN	543	66.683	-3.903	19.507	1.00	29.12
ATOM	4170	CA	ASN	543	65.425	-3.012	21.446	1.00	28.54
ATOM	4171	CB	ASN	543	64.245	-2.559	20.869	1.00	29.10
ATOM	4172	CG	ASN	543	64.253	-3.047	21.712	1.00	29.69
ATOM	4173	OD1	ASN	543	64.510	-4.556	21.900	1.00	29.62
ATOM	4174	ND2	ASN	543	64.020	-5.050	23.000	1.00	31.63
ATOM	4177	C	ASN	543	65.299	-5.291	20.828	1.00	28.66
ATOM	4178	O	ASN	543	64.207	-1.073	20.532	1.00	29.61
ATOM	4179	N	ILE	544	66.432	-0.507	20.578	1.00	28.00
ATOM	4181	CA	ILE	544	66.466	-0.442	20.222	1.00	28.39
ATOM	4182	CB	ILE	544	66.903	0.958	19.804	1.00	25.73
ATOM	4183	CG2	ILE	544	66.083	1.952	20.935	1.00	25.98
ATOM	4184	CG1	ILE	544	68.412	1.721	22.215	1.00	22.04
ATOM	4185	CD1	ILE	544	68.901	1.860	21.209	1.00	24.30
ATOM	4186	C	ILE	544	67.463	2.846	22.274	1.00	22.83
ATOM	4187	O	ILE	544	68.276	1.020	18.639	1.00	26.20
ATOM	4188	N	ILE	545	67.307	0.106	18.467	1.00	25.46
ATOM	4190	CA	ILE	545	68.223	2.016	17.771	1.00	26.26
ATOM	4191	CB	ILE	545	67.647	2.209	16.641	1.00	27.62
ATOM	4192	CG2	ILE	545	68.726	3.195	15.585	1.00	28.33
ATOM	4193	CG1	ILE	545	66.453	3.595	14.562	1.00	28.00
ATOM	4194	CD1	ILE	545	66.850	2.565	14.856	1.00	24.69
ATOM	4195	C	ILE	545	69.492	1.467	13.875	1.00	26.17
ATOM	4196	O	ILE	545	69.468	2.794	17.267	1.00	28.23
ATOM	4197	N	ASN	546	70.595	3.872	17.846	1.00	28.97
ATOM	4199	CA	ASN	546	71.845	2.069	17.164	1.00	29.45
ATOM	4200	CB	ASN	546	72.580	2.508	17.774	1.00	28.58
ATOM	4201	CG	ASN	546	71.812	1.309	18.384	1.00	26.34
ATOM	4202	OD1	ASN	546	71.634	0.673	19.527	1.00	25.52
ATOM	4203	ND2	ASN	546	71.341	1.277	20.580	1.00	28.82
ATOM	4206	C	ASN	546	72.810	-0.542	19.318	1.00	26.57
ATOM	4207	O	ASN	546	72.858	3.264	16.881	1.00	28.74
ATOM	4208	N	LEU	547	73.578	3.041	15.675	1.00	29.26
ATOM	4210	CA	LEU	547	74.618	4.155	17.504	1.00	29.90
ATOM	4211	CB	LEU	547	75.075	4.936	16.834	1.00	30.27
						6.081	17.745	1.00	25.85

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ATOM	4212	CG	LEU	547	76.161	7.034	17.232	1.00	27.73
ATOM	4213	CD1	LEU	547	75.670	7.851	16.033	1.00	27.38
ATOM	4214	CD2	LEU	547	76.545	7.966	18.345	1.00	29.14
ATOM	4215	C	LEU	547	75.811	4.004	16.567	1.00	32.22
ATOM	4216	O	LEU	547	76.256	3.291	17.471	1.00	33.38
ATOM	4217	N	LEU	548	76.317	4.005	15.335	1.00	32.12
ATOM	4219	CA	LEU	548	77.452	3.159	14.960	1.00	32.94
ATOM	4220	CB	LEU	548	77.103	2.310	13.740	1.00	29.97
ATOM	4221	CG	LEU	548	75.839	1.458	13.840	1.00	31.55
ATOM	4222	CD1	LEU	548	75.662	0.713	12.540	1.00	27.85
ATOM	4223	CD2	LEU	548	75.917	0.500	15.025	1.00	26.34
ATOM	4224	C	LEU	548	78.726	3.955	14.654	1.00	36.06
ATOM	4225	O	LEU	548	79.836	3.410	14.668	1.00	36.42
ATOM	4226	N	GLY	549	78.562	5.219	14.298	1.00	35.78
ATOM	4228	CA	GLY	549	79.713	6.042	13.987	1.00	36.22
ATOM	4229	C	GLY	549	79.267	7.376	13.433	1.00	35.30
ATOM	4230	O	GLY	549	78.062	7.646	13.362	1.00	33.46
ATOM	4231	N	ALA	550	80.232	8.206	13.042	1.00	34.94
ATOM	4233	CA	ALA	550	79.945	9.525	12.490	1.00	31.91
ATOM	4234	CB	ALA	550	79.588	10.495	13.613	1.00	30.54
ATOM	4235	C	ALA	550	81.128	10.077	11.715	1.00	31.58
ATOM	4236	O	ALA	550	82.281	9.832	12.080	1.00	31.23
ATOM	4237	N	CYS	551	80.818	10.812	10.643	1.00	31.13
ATOM	4239	CA	CYS	551	81.805	11.503	9.804	1.00	28.28
ATOM	4240	CB	CYS	551	81.621	11.180	8.316	1.00	27.27
ATOM	4241	SG	CYS	551	81.771	9.449	7.839	1.00	30.33
ATOM	4242	C	CYS	551	81.450	12.960	10.074	1.00	25.88
ATOM	4243	O	CYS	551	80.432	13.458	9.605	1.00	27.73
ATOM	4244	N	THR	552	82.214	13.586	10.954	1.00	25.35
ATOM	4246	CA	THR	552	81.988	14.967	11.353	1.00	26.79
ATOM	4247	CB	THR	552	82.051	15.092	12.899	1.00	27.76
ATOM	4248	OG1	THR	552	83.392	14.839	13.338	1.00	27.62
ATOM	4250	CG2	THR	552	81.119	14.086	13.575	1.00	29.17
ATOM	4251	C	THR	552	83.036	15.931	10.790	1.00	25.03
ATOM	4252	O	THR	552	82.825	17.137	10.746	1.00	25.34
ATOM	4253	N	GLN	553	84.174	15.385	10.381	1.00	27.34
ATOM	4255	CA	GLN	553	85.285	16.190	9.888	1.00	26.31
ATOM	4256	CB	GLN	553	86.601	15.639	10.468	1.00	25.05
ATOM	4257	CG	GLN	553	86.581	15.491	11.993	1.00	24.78
ATOM	4258	CD	GLN	553	86.382	16.823	12.709	1.00	25.40
ATOM	4259	OE1	GLN	553	87.175	17.748	12.546	1.00	33.74
ATOM	4260	NE2	GLN	553	85.338	16.920	13.516	1.00	25.61
ATOM	4263	C	GLN	553	85.390	16.274	8.379	1.00	27.08
ATOM	4264	O	GLN	553	85.083	15.318	7.669	1.00	28.76
ATOM	4265	N	ASP	554	85.804	17.438	7.899	1.00	28.63
ATOM	4267	CA	ASP	554	86.015	17.677	6.471	1.00	29.70
ATOM	4268	CB	ASP	554	87.335	17.050	6.051	1.00	29.73
ATOM	4269	CG	ASP	554	88.480	17.587	6.857	1.00	33.38
ATOM	4270	OD1	ASP	554	88.794	18.780	6.711	1.00	36.53
ATOM	4271	OD2	ASP	554	89.024	16.841	7.687	1.00	36.40
ATOM	4272	C	ASP	554	84.908	17.258	5.522	1.00	29.64
ATOM	4273	O	ASP	554	85.112	16.422	4.643	1.00	32.06
ATOM	4274	N	GLY	555	83.748	17.881	5.679	1.00	28.59
ATOM	4276	CA	GLY	555	82.620	17.579	4.825	1.00	26.85

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ATOM	4277	C	GLY	555	81.333	17.434	5.607	1.00	25.30
ATOM	4278	O	GLY	555	81.319	17.593	6.834	1.00	23.96
ATOM	4279	N	PRO	556	80.229	17.113	4.920	1.00	24.84
ATOM	4280	CD	PRO	556	80.159	16.850	3.472	1.00	21.36
ATOM	4281	CA	PRO	556	78.920	16.942	5.550	1.00	25.26
ATOM	4282	CB	PRO	556	78.033	16.494	4.386	1.00	23.37
ATOM	4283	CG	PRO	556	79.025	15.881	3.398	1.00	24.44
ATOM	4284	C	PRO	556	78.885	15.941	6.700	1.00	26.50
ATOM	4285	O	PRO	556	79.515	14.875	6.654	1.00	27.38
ATOM	4286	N	LEU	557	78.171	16.314	7.754	1.00	26.25
ATOM	4288	CA	LEU	557	78.032	15.452	8.917	1.00	28.25
ATOM	4289	CB	LEU	557	77.403	16.217	10.092	1.00	27.09
ATOM	4290	CG	LEU	557	76.922	15.414	11.310	1.00	28.35
ATOM	4291	CD1	LEU	557	78.088	14.733	12.011	1.00	25.54
ATOM	4292	CD2	LEU	557	76.204	16.340	12.271	1.00	26.91
ATOM	4293	C	LEU	557	77.169	14.246	8.554	1.00	29.06
ATOM	4294	O	LEU	557	76.060	14.385	8.011	1.00	29.05
ATOM	4295	N	TYR	558	77.717	13.065	8.807	1.00	29.43
ATOM	4297	CA	TYR	558	77.018	11.823	8.573	1.00	28.02
ATOM	4298	CB	TYR	558	77.813	10.918	7.632	1.00	27.83
ATOM	4299	CG	TYR	558	77.969	11.414	6.203	1.00	31.70
ATOM	4300	CD1	TYR	558	78.966	10.893	5.383	1.00	32.90
ATOM	4301	CE1	TYR	558	79.121	11.315	4.073	1.00	32.69
ATOM	4302	CD2	TYR	558	77.122	12.386	5.666	1.00	30.23
ATOM	4303	CE2	TYR	558	77.271	12.815	4.350	1.00	29.97
ATOM	4304	CZ	TYR	558	78.280	12.272	3.560	1.00	33.20
ATOM	4305	OH	TYR	558	78.452	12.681	2.253	1.00	35.32
ATOM	4307	C	TYR	558	76.848	11.131	9.932	1.00	28.42
ATOM	4308	O	TYR	558	77.823	10.902	10.647	1.00	27.81
ATOM	4309	N	VAL	559	75.601	10.870	10.313	1.00	29.20
ATOM	4311	CA	VAL	559	75.286	10.175	11.564	1.00	29.17
ATOM	4312	CB	VAL	559	74.102	10.832	12.329	1.00	28.53
ATOM	4313	CG1	VAL	559	73.802	10.036	13.607	1.00	27.08
ATOM	4314	CG2	VAL	559	74.456	12.281	12.687	1.00	23.27
ATOM	4315	C	VAL	559	74.911	8.772	11.137	1.00	26.41
ATOM	4316	O	VAL	559	73.834	8.536	10.593	1.00	25.91
ATOM	4317	N	ILE	560	75.824	7.846	11.371	1.00	26.71
ATOM	4319	CA	ILE	560	75.638	6.465	10.966	1.00	27.55
ATOM	4320	CB	ILE	560	77.012	5.829	10.619	1.00	28.48
ATOM	4321	CG2	ILE	560	76.819	4.468	9.979	1.00	29.18
ATOM	4322	CG1	ILE	560	77.793	6.745	9.657	1.00	27.99
ATOM	4323	CD1	ILE	560	79.274	6.399	9.525	1.00	28.97
ATOM	4324	C	ILE	560	74.917	5.644	12.034	1.00	29.17
ATOM	4325	O	ILE	560	75.404	5.497	13.160	1.00	28.92
ATOM	4326	N	VAL	561	73.743	5.129	11.681	1.00	28.60
ATOM	4328	CA	VAL	561	72.957	4.325	12.606	1.00	28.58
ATOM	4329	CB	VAL	561	71.634	5.061	13.047	1.00	27.53
ATOM	4330	CG1	VAL	561	71.951	6.400	13.701	1.00	22.44
ATOM	4331	CG2	VAL	561	70.697	5.246	11.874	1.00	23.19
ATOM	4332	C	VAL	561	72.618	2.956	12.006	1.00	28.20
ATOM	4333	O	VAL	561	72.875	2.694	10.825	1.00	27.99
ATOM	4334	N	GLU	562	72.057	2.079	12.834	1.00	29.17
ATOM	4336	CA	GLU	562	71.666	0.744	12.399	1.00	28.96
ATOM	4337	CB	GLU	562	71.199	-0.086	13.589	1.00	27.34

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ATOM	4338	CG	GLU	562	72.308	-0.331	14.583	1.00	30.12
ATOM	4339	CD	GLU	562	71.838	-1.075	15.808	1.00	32.29
ATOM	4340	OE1	GLU	562	72.526	-2.030	16.217	1.00	32.45
ATOM	4341	OE2	GLU	562	70.785	-0.702	16.362	1.00	30.16
ATOM	4342	C	GLU	562	70.580	0.794	11.340	1.00	29.79
ATOM	4343	O	GLU	562	69.690	1.653	11.386	1.00	29.75
ATOM	4344	N	TYR	563	70.684	-0.106	10.369	1.00	30.51
ATOM	4346	CA	TYR	563	69.735	-0.209	9.267	1.00	33.76
ATOM	4347	CB	TYR	563	70.494	-0.602	7.988	1.00	31.04
ATOM	4348	CG	TYR	563	69.624	-0.928	6.806	1.00	33.40
ATOM	4349	CD1	TYR	563	68.693	-0.019	6.340	1.00	33.07
ATOM	4350	CE1	TYR	563	67.908	-0.301	5.240	1.00	34.71
ATOM	4351	CD2	TYR	563	69.749	-2.141	6.147	1.00	34.61
ATOM	4352	CE2	TYR	563	68.970	-2.446	5.035	1.00	36.54
ATOM	4353	CZ	TYR	563	68.047	-1.518	4.589	1.00	36.83
ATOM	4354	OH	TYR	563	67.261	-1.805	3.501	1.00	38.81
ATOM	4356	C	TYR	563	68.655	-1.269	9.588	1.00	36.14
ATOM	4357	O	TYR	563	68.946	-2.365	10.023	1.00	37.70
ATOM	4358	N	ALA	564	67.406	-0.948	9.309	1.00	37.87
ATOM	4360	CA	ALA	564	66.276	-1.832	9.534	1.00	38.49
ATOM	4361	CB	ALA	564	65.278	-1.167	10.458	1.00	42.57
ATOM	4362	C	ALA	564	65.645	-2.153	8.179	1.00	39.65
ATOM	4363	O	ALA	564	64.796	-1.423	7.687	1.00	39.74
ATOM	4364	N	SER	565	66.039	-3.280	7.607	1.00	40.06
ATOM	4366	CA	SER	565	65.567	-3.699	6.295	1.00	40.67
ATOM	4367	CB	SER	565	66.267	-4.986	5.883	1.00	38.71
ATOM	4368	OG	SER	565	66.107	-5.964	6.889	1.00	41.35
ATOM	4370	C	SER	565	64.081	-3.884	6.106	1.00	42.17
ATOM	4371	O	SER	565	63.585	-3.741	4.992	1.00	44.25
ATOM	4372	N	LYS	566	63.360	-4.207	7.167	1.00	41.71
ATOM	4374	CA	LYS	566	61.928	-4.427	7.015	1.00	40.22
ATOM	4375	CB	LYS	566	61.525	-5.668	7.800	1.00	39.51
ATOM	4376	CG	LYS	566	62.202	-6.910	7.226	1.00	41.48
ATOM	4377	CD	LYS	566	62.113	-8.094	8.149	1.00	41.53
ATOM	4378	CE	LYS	566	62.710	-9.312	7.491	1.00	41.18
ATOM	4379	NZ	LYS	566	62.763	-10.458	8.438	1.00	46.17
ATOM	4383	C	LYS	566	61.007	-3.220	7.263	1.00	40.47
ATOM	4384	O	LYS	566	59.800	-3.367	7.486	1.00	42.68
ATOM	4385	N	GLY	567	61.584	-2.026	7.167	1.00	38.90
ATOM	4387	CA	GLY	567	60.826	-0.799	7.336	1.00	37.13
ATOM	4388	C	GLY	567	60.199	-0.592	8.694	1.00	36.72
ATOM	4389	O	GLY	567	60.644	-1.172	9.683	1.00	38.48
ATOM	4390	N	ASN	568	59.191	0.273	8.753	1.00	35.77
ATOM	4392	CA	ASN	568	58.518	0.549	10.015	1.00	35.36
ATOM	4393	CB	ASN	568	57.883	1.957	10.045	1.00	36.30
ATOM	4394	CG	ASN	568	56.635	2.088	9.169	1.00	38.06
ATOM	4395	OD1	ASN	568	55.623	1.421	9.383	1.00	38.66
ATOM	4396	ND2	ASN	568	56.686	3.010	8.221	1.00	37.29
ATOM	4399	C	ASN	568	57.504	-0.532	10.341	1.00	33.04
ATOM	4400	O	ASN	568	57.061	-1.265	9.461	1.00	32.10
ATOM	4401	N	LEU	569	57.142	-0.612	11.617	1.00	33.59
ATOM	4403	CA	LEU	569	56.199	-1.604	12.132	1.00	32.91
ATOM	4404	CB	LEU	569	56.045	-1.428	13.647	1.00	33.84
ATOM	4405	CG	LEU	569	55.088	-2.343	14.403	1.00	31.96

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ATOM	4406	CD1	LEU	569	55.522	-3.797	14.216	1.00	33.20
ATOM	4407	CD2	LEU	569	55.089	-1.967	15.868	1.00	30.81
ATOM	4408	C	LEU	569	54.820	-1.591	11.478	1.00	32.12
ATOM	4409	O	LEU	569	54.214	-2.645	11.300	1.00	33.08
ATOM	4410	N	ARG	570	54.315	-0.409	11.148	1.00	32.05
ATOM	4412	CA	ARG	570	52.999	-0.293	10.529	1.00	35.21
ATOM	4413	CB	ARG	570	52.659	1.173	10.256	1.00	36.77
ATOM	4414	CG	ARG	570	51.282	1.370	9.653	1.00	43.11
ATOM	4415	CD	ARG	570	51.203	2.690	8.926	1.00	49.24
ATOM	4416	NE	ARG	570	52.154	2.775	7.815	1.00	55.77
ATOM	4418	CZ	ARG	570	52.995	3.790	7.619	1.00	58.89
ATOM	4419	NH1	ARG	570	53.016	4.820	8.463	1.00	61.61
ATOM	4422	NH2	ARG	570	53.804	3.786	6.566	1.00	59.16
ATOM	4425	C	ARG	570	52.992	-1.063	9.220	1.00	35.16
ATOM	4426	O	ARG	570	52.145	-1.922	8.990	1.00	35.50
ATOM	4427	N	GLU	571	53.971	-0.760	8.383	1.00	36.29
ATOM	4429	CA	GLU	571	54.111	-1.400	7.089	1.00	37.51
ATOM	4430	CB	GLU	571	55.219	-0.701	6.308	1.00	41.27
ATOM	4431	CG	GLU	571	54.945	0.778	6.110	1.00	49.88
ATOM	4432	CD	GLU	571	56.087	1.516	5.436	1.00	57.58
ATOM	4433	OE1	GLU	571	57.264	-1.122	5.636	1.00	60.59
ATOM	4434	OE2	GLU	571	55.804	2.504	4.714	1.00	61.14
ATOM	4435	C	GLU	571	54.399	-2.896	7.228	1.00	36.24
ATOM	4436	O	GLU	571	53.889	-3.716	6.459	1.00	34.22
ATOM	4437	N	TYR	572	55.202	-3.238	8.232	1.00	35.98
ATOM	4439	CA	TYR	572	55.570	-4.619	8.517	1.00	35.34
ATOM	4440	CB	TYR	572	56.526	-4.656	9.714	1.00	30.94
ATOM	4441	CG	TYR	572	56.959	-6.034	10.180	1.00	32.71
ATOM	4442	CD1	TYR	572	58.009	-6.714	9.547	1.00	32.33
ATOM	4443	CE1	TYR	572	58.464	-7.940	10.026	1.00	30.31
ATOM	4444	CD2	TYR	572	56.369	-6.626	11.303	1.00	33.43
ATOM	4445	CE2	TYR	572	56.813	-7.851	11.791	1.00	31.46
ATOM	4446	CZ	TYR	572	57.864	-8.502	11.148	1.00	33.99
ATOM	4447	OH	TYR	572	58.311	-9.706	11.640	1.00	36.30
ATOM	4449	C	TYR	572	54.312	-5.425	8.826	1.00	37.26
ATOM	4450	O	TYR	572	54.121	-6.530	8.314	1.00	36.91
ATOM	4451	N	LEU	573	53.457	-4.850	9.665	1.00	36.82
ATOM	4453	CA	LEU	573	52.208	-5.476	10.075	1.00	35.56
ATOM	4454	CB	LEU	573	51.537	-4.629	11.165	1.00	34.03
ATOM	4455	CG	LEU	573	52.238	-4.527	12.519	1.00	32.82
ATOM	4456	CD1	LEU	573	51.621	-3.423	13.377	1.00	28.95
ATOM	4457	CD2	LEU	573	52.168	-5.858	13.207	1.00	29.46
ATOM	4458	C	LEU	573	51.237	-5.658	8.915	1.00	34.56
ATOM	4459	O	LEU	573	50.670	-6.729	8.726	1.00	34.80
ATOM	4460	N	GLN	574	51.030	-4.602	8.150	1.00	37.10
ATOM	4462	CA	GLN	574	50.101	-4.666	7.031	1.00	41.15
ATOM	4463	CB	GLN	574	49.875	-3.278	6.457	1.00	41.63
ATOM	4464	CG	GLN	574	49.089	-2.375	7.366	1.00	43.13
ATOM	4465	CD	GLN	574	49.063	-0.959	6.860	1.00	47.77
ATOM	4466	OE1	GLN	574	49.655	-0.647	5.827	1.00	50.00
ATOM	4467	NE2	GLN	574	48.378	-0.086	7.582	1.00	49.67
ATOM	4470	C	GLN	574	50.529	-5.627	5.934	1.00	42.38
ATOM	4471	O	GLN	574	49.685	-6.284	5.318	1.00	44.56
ATOM	4472	N	ALA	575	51.835	-5.717	5.697	1.00	41.99

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ATOM	4474	CA	ALA	575	52.367	-6.608	4.676	1.00	41.29
ATOM	4475	CB	ALA	575	53.841	-6.325	4.446	1.00	40.43
ATOM	4476	C	ALA	575	52.186	-8.058	5.066	1.00	41.42
ATOM	4477	O	ALA	575	52.392	-8.949	4.249	1.00	43.65
ATOM	4478	N	ARG	576	51.815	-8.294	6.319	1.00	42.56
ATOM	4480	CA	ARG	576	51.642	-9.646	6.824	1.00	42.51
ATOM	4481	CB	ARG	576	52.676	-9.910	7.920	1.00	40.14
ATOM	4482	CG	ARG	576	54.100	-9.896	7.377	1.00	40.32
ATOM	4483	CD	ARG	576	55.172	-9.836	8.460	1.00	40.78
ATOM	4484	NE	ARG	576	56.513	-9.783	7.874	1.00	42.13
ATOM	4486	CZ	ARG	576	56.975	-8.785	7.120	1.00	40.73
ATOM	4487	NH1	ARG	576	56.215	-7.732	6.851	1.00	39.21
ATOM	4490	NH2	ARG	576	58.201	-8.846	6.622	1.00	37.62
ATOM	4493	C	ARG	576	50.242	-9.931	7.326	1.00	44.48
ATOM	4494	O	ARG	576	50.028	-10.869	8.098	1.00	46.84
ATOM	4495	N	ARG	577	49.275	-9.146	6.866	1.00	46.26
ATOM	4497	CA	ARG	577	47.893	-9.344	7.292	1.00	46.89
ATOM	4498	CB	ARG	577	47.027	-8.170	6.845	1.00	46.16
ATOM	4499	CG	ARG	577	47.189	-6.939	7.696	1.00	44.93
ATOM	4500	CD	ARG	577	46.463	-5.766	7.080	1.00	44.60
ATOM	4501	NE	ARG	577	46.284	-4.683	8.039	1.00	45.05
ATOM	4503	CZ	ARG	577	45.612	-3.565	7.793	1.00	45.95
ATOM	4504	NH1	ARG	577	45.052	-3.372	6.606	1.00	47.39
ATOM	4507	NH2	ARG	577	45.466	-2.655	8.749	1.00	45.49
ATOM	4510	C	ARG	577	47.334	-10.649	6.740	1.00	46.60
ATOM	4511	O	ARG	577	47.478	-10.933	5.551	1.00	47.15
ATOM	4512	N	GLN	594	53.312	-14.007	7.967	1.00	63.97
ATOM	4514	CA	GLN	594	52.110	-14.068	8.799	1.00	63.06
ATOM	4515	CB	GLN	594	51.175	-15.183	8.319	1.00	64.16
ATOM	4516	C	GLN	594	52.501	-14.278	10.258	1.00	61.68
ATOM	4517	O	GLN	594	53.101	-15.292	10.619	1.00	60.95
ATOM	4518	N	LEU	595	52.140	-13.313	11.092	1.00	58.58
ATOM	4520	CA	LEU	595	52.470	-13.335	12.505	1.00	55.58
ATOM	4521	CB	LEU	595	52.619	-11.902	13.020	1.00	54.05
ATOM	4522	CG	LEU	595	53.570	-11.074	12.153	1.00	56.23
ATOM	4523	CD1	LEU	595	53.496	-9.609	12.524	1.00	58.84
ATOM	4524	CD2	LEU	595	54.977	-11.596	12.301	1.00	55.93
ATOM	4525	C	LEU	595	51.480	-14.093	13.372	1.00	53.77
ATOM	4526	O	LEU	595	50.276	-14.046	13.139	1.00	54.31
ATOM	4527	N	SER	596	52.012	-14.780	14.377	1.00	51.04
ATOM	4529	CA	SER	596	51.206	-15.541	15.316	1.00	48.97
ATOM	4530	CB	SER	596	52.004	-16.737	15.834	1.00	48.89
ATOM	4531	OG	SER	596	52.945	-16.345	16.820	1.00	48.59
ATOM	4533	C	SER	596	50.853	-14.641	16.488	1.00	47.56
ATOM	4534	O	SER	596	51.470	-13.590	16.676	1.00	46.71
ATOM	4535	N	SER	597	49.888	-15.070	17.292	1.00	47.11
ATOM	4537	CA	SER	597	49.462	-14.315	18.461	1.00	47.88
ATOM	4538	CB	SER	597	48.386	-15.084	19.229	1.00	50.66
ATOM	4539	OG	SER	597	47.574	-15.839	18.343	1.00	57.08
ATOM	4541	C	SER	597	50.666	-14.068	19.372	1.00	46.03
ATOM	4542	O	SER	597	50.735	-13.045	20.047	1.00	46.49
ATOM	4543	N	LYS	598	51.607	-15.007	19.399	1.00	46.08
ATOM	4545	CA	LYS	598	52.798	-14.844	20.229	1.00	46.33
ATOM	4546	CB	LYS	598	53.558	-16.163	20.384	1.00	46.67

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ATOM	4547	CG	LYS	598	54.449	-16.224	21.623	1.00	49.61
ATOM	4548	CD	LYS	598	55.240	-17.539	21.668	1.00	53.69
ATOM	4549	CE	LYS	598	55.899	-17.797	23.026	1.00	53.15
ATOM	4550	NZ	LYS	598	54.891	-18.076	24.093	1.00	52.02
ATOM	4554	C	LYS	598	53.706	-13.790	19.599	1.00	45.43
ATOM	4555	O	LYS	598	54.292	-12.968	20.311	1.00	44.18
ATOM	4556	N	ASP	599	53.780	-13.804	18.264	1.00	44.16
ATOM	4558	CA	ASP	599	54.598	-12.851	17.513	1.00	43.46
ATOM	4559	CB	ASP	599	54.523	-13.098	16.001	1.00	44.83
ATOM	4560	CG	ASP	599	55.288	-14.336	15.560	1.00	48.24
ATOM	4561	OD1	ASP	599	56.228	-14.754	16.260	1.00	52.90
ATOM	4562	OD2	ASP	599	54.958	-14.894	14.493	1.00	51.43
ATOM	4563	C	ASP	599	54.120	-11.437	17.796	1.00	42.71
ATOM	4564	O	ASP	599	54.937	-10.550	18.059	1.00	45.00
ATOM	4565	N	LEU	600	52.803	-11.235	17.776	1.00	37.69
ATOM	4567	CA	LEU	600	52.246	-9.918	18.030	1.00	34.03
ATOM	4568	CB	LEU	600	50.747	-9.882	17.747	1.00	34.06
ATOM	4569	CG	LEU	600	50.332	-10.068	16.281	1.00	33.13
ATOM	4570	CD1	LEU	600	48.814	-9.992	16.190	1.00	37.38
ATOM	4571	CD2	LEU	600	50.974	-9.012	15.373	1.00	25.63
ATOM	4572	C	LEU	600	52.537	-9.452	19.439	1.00	34.58
ATOM	4573	O	LEU	600	52.910	-8.294	19.636	1.00	33.18
ATOM	4574	N	VAL	601	52.415	-10.348	20.419	1.00	34.24
ATOM	4576	CA	VAL	601	52.692	-9.969	21.808	1.00	35.80
ATOM	4577	CB	VAL	601	52.214	-11.036	22.827	1.00	37.50
ATOM	4578	CG1	VAL	601	52.331	-10.483	24.252	1.00	38.08
ATOM	4579	CG2	VAL	601	50.766	-11.409	22.560	1.00	40.77
ATOM	4580	C	VAL	601	54.198	-9.741	21.982	1.00	35.04
ATOM	4581	O	VAL	601	54.634	-8.856	22.731	1.00	34.33
ATOM	4582	N	SER	602	54.981	-10.531	21.262	1.00	32.58
ATOM	4584	CA	SER	602	56.421	-10.421	21.307	1.00	36.01
ATOM	4585	CB	SER	602	57.045	-11.504	20.439	1.00	38.43
ATOM	4586	OG	SER	602	58.453	-11.387	20.419	1.00	43.36
ATOM	4588	C	SER	602	56.809	-9.038	20.800	1.00	35.21
ATOM	4589	O	SER	602	57.651	-8.363	21.394	1.00	35.03
ATOM	4590	N	CYS	603	56.183	-8.614	19.707	1.00	34.15
ATOM	4592	CA	CYS	603	56.438	-7.294	19.141	1.00	34.04
ATOM	4593	CB	CYS	603	55.543	-7.055	17.925	1.00	33.45
ATOM	4594	SG	CYS	603	55.653	-5.423	17.229	0.50	32.19
ATOM	4595	C	CYS	603	56.198	-6.211	20.191	1.00	32.79
ATOM	4596	O	CYS	603	57.023	-5.316	20.362	1.00	33.36
ATOM	4597	N	ALA	604	55.088	-6.321	20.917	1.00	31.31
ATOM	4599	CA	ALA	604	54.743	-5.358	21.965	1.00	32.36
ATOM	4600	CB	ALA	604	53.321	-5.610	22.481	1.00	32.01
ATOM	4601	C	ALA	604	55.741	-5.394	23.128	1.00	32.83
ATOM	4602	O	ALA	604	56.050	-4.358	23.727	1.00	30.89
ATOM	4603	N	TYR	605	56.212	-6.592	23.465	1.00	32.95
ATOM	4605	CA	TYR	605	57.189	-6.758	24.539	1.00	33.34
ATOM	4606	CB	TYR	605	57.500	-8.236	24.737	1.00	32.58
ATOM	4607	CG	TYR	605	58.640	-8.495	25.690	1.00	32.51
ATOM	4608	CD1	TYR	605	58.511	-8.236	27.053	1.00	33.50
ATOM	4609	CE1	TYR	605	59.556	-8.507	27.943	1.00	37.08
ATOM	4610	CD2	TYR	605	59.841	-9.026	25.230	1.00	34.22
ATOM	4611	CE2	TYR	605	60.896	-9.300	26.109	1.00	36.64

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ATOM	4612	CZ	TYR	605	60.746	-9.042	27.464	1.00	37.56
ATOM	4613	OH	TYR	605	61.776	-9.342	28.336	1.00	38.08
ATOM	4615	C	TYR	605	58.480	-6.006	24.191	1.00	32.42
ATOM	4616	O	TYR	605	58.975	-5.203	24.991	1.00	33.34
ATOM	4617	N	GLN	606	58.997	-6.267	22.989	1.00	30.61
ATOM	4619	CA	GLN	606	60.218	-5.643	22.474	1.00	31.12
ATOM	4620	CB	GLN	606	60.499	-6.143	21.058	1.00	30.57
ATOM	4621	CG	GLN	606	61.044	-7.568	21.008	1.00	33.90
ATOM	4622	CD	GLN	606	61.240	-8.080	19.593	1.00	32.17
ATOM	4623	OE1	GLN	606	62.155	-7.652	18.883	1.00	32.55
ATOM	4624	NE2	GLN	606	60.374	-8.998	19.171	1.00	33.10
ATOM	4627	C	GLN	606	60.157	-4.114	22.487	1.00	31.69
ATOM	4628	O	GLN	606	61.111	-3.453	22.910	1.00	31.18
ATOM	4629	N	VAL	607	59.035	-3.564	22.020	1.00	29.50
ATOM	4631	CA	VAL	607	58.816	-2.122	22.000	1.00	27.54
ATOM	4632	CB	VAL	607	57.454	-1.751	21.306	1.00	26.79
ATOM	4633	CG1	VAL	607	57.131	-0.291	21.516	1.00	24.80
ATOM	4634	CG2	VAL	607	57.505	-2.050	19.815	1.00	22.95
ATOM	4635	C	VAL	607	58.827	-1.576	23.432	1.00	28.30
ATOM	4636	O	VAL	607	59.469	-0.548	23.705	1.00	28.32
ATOM	4637	N	ALA	608	58.110	-2.247	24.340	1.00	27.21
ATOM	4639	CA	ALA	608	58.061	-1.805	25.735	1.00	26.54
ATOM	4640	CB	ALA	608	57.070	-2.649	26.550	1.00	26.70
ATOM	4641	C	ALA	608	59.457	-1.850	26.368	1.00	25.97
ATOM	4642	O	ALA	608	59.802	-0.993	27.183	1.00	25.88
ATOM	4643	N	ARG	609	60.250	-2.848	25.994	1.00	26.02
ATOM	4645	CA	ARG	609	61.606	-2.977	26.512	1.00	30.44
ATOM	4646	CB	ARG	609	62.234	-4.285	26.058	1.00	34.09
ATOM	4647	CG	ARG	609	61.642	-5.516	26.682	1.00	39.24
ATOM	4648	CD	ARG	609	62.659	-6.615	26.615	1.00	42.75
ATOM	4649	NE	ARG	609	63.405	-6.704	27.860	1.00	45.52
ATOM	4651	CZ	ARG	609	64.525	-7.405	28.019	1.00	46.24
ATOM	4652	NH1	ARG	609	65.055	-8.079	27.001	1.00	41.48
ATOM	4655	NH2	ARG	609	65.079	-7.482	29.225	1.00	47.49
ATOM	4658	C	ARG	609	62.478	-1.829	26.015	1.00	34.20
ATOM	4659	O	ARG	609	63.265	-1.255	26.788	1.00	35.24
ATOM	4660	N	GLY	610	62.368	-1.528	24.717	1.00	33.25
ATOM	4662	CA	GLY	610	63.130	-0.439	24.138	1.00	29.57
ATOM	4663	C	GLY	610	62.802	0.814	24.908	1.00	29.31
ATOM	4664	O	GLY	610	63.695	1.543	25.335	1.00	27.46
ATOM	4665	N	MET	611	61.507	1.020	25.147	1.00	31.07
ATOM	4667	CA	MET	611	61.016	2.178	25.889	1.00	30.09
ATOM	4668	CB	MET	611	59.493	2.280	25.782	1.00	29.51
ATOM	4669	CG	MET	611	58.997	2.655	24.404	1.00	28.21
ATOM	4670	SD	MET	611	59.760	4.175	23.787	1.00	29.00
ATOM	4671	CE	MET	611	59.350	5.335	25.039	1.00	25.91
ATOM	4672	C	MET	611	61.439	2.189	27.361	1.00	30.47
ATOM	4673	O	MET	611	61.734	3.242	27.919	1.00	29.43
ATOM	4674	N	GLU	612	61.429	1.031	28.002	1.00	31.97
ATOM	4676	CA	GLU	612	61.836	0.947	29.402	1.00	35.34
ATOM	4677	CB	GLU	612	61.707	-0.490	29.904	1.00	36.17
ATOM	4678	CG	GLU	612	62.305	-0.729	31.278	1.00	34.87
ATOM	4679	CD	GLU	612	62.259	-2.185	31.705	1.00	32.68
ATOM	4680	OE1	GLU	612	62.641	-3.070	30.904	1.00	35.01

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ATOM	4681	OE2	GLU	612	61.848	-2.443	32.858	1.00	36.56
ATOM	4682	C	GLU	612	63.296	1.425	29.490	1.00	35.26
ATOM	4683	O	GLU	612	63.677	2.162	30.417	1.00	31.21
ATOM	4684	N	TYR	613	64.092	1.040	28.491	1.00	36.10
ATOM	4686	CA	TYR	613	65.491	1.458	28.440	1.00	34.76
ATOM	4687	CB	TYR	613	66.249	0.788	27.301	1.00	31.15
ATOM	4688	CG	TYR	613	67.700	1.195	27.284	1.00	34.28
ATOM	4689	CD1	TYR	613	68.600	0.654	28.207	1.00	36.50
ATOM	4690	CE1	TYR	613	69.949	1.035	28.219	1.00	38.20
ATOM	4691	CD2	TYR	613	68.179	2.135	26.366	1.00	32.99
ATOM	4692	CE2	TYR	613	69.520	2.526	26.372	1.00	33.32
ATOM	4693	CZ	TYR	613	70.399	1.968	27.302	1.00	36.59
ATOM	4694	OH	TYR	613	71.721	2.340	27.333	1.00	35.73
ATOM	4696	C	TYR	613	65.583	2.970	28.273	1.00	34.03
ATOM	4697	O	TYR	613	66.231	3.643	29.075	1.00	35.26
ATOM	4698	N	LEU	614	64.916	3.503	27.250	1.00	31.78
ATOM	4700	CA	LEU	614	64.945	4.937	26.998	1.00	29.50
ATOM	4701	CB	LEU	614	64.095	5.297	25.775	1.00	28.26
ATOM	4702	CG	LEU	614	64.564	4.742	24.422	1.00	31.29
ATOM	4703	CD1	LEU	614	63.564	5.089	23.321	1.00	28.09
ATOM	4704	CD2	LEU	614	65.951	5.282	24.079	1.00	29.52
ATOM	4705	C	LEU	614	64.489	5.715	28.224	1.00	32.49
ATOM	4706	O	LEU	614	65.108	6.717	28.598	1.00	31.73
ATOM	4707	N	ALA	615	63.431	5.232	28.872	1.00	33.06
ATOM	4709	CA	ALA	615	62.906	5.870	30.070	1.00	35.16
ATOM	4710	CB	ALA	615	61.598	5.192	30.511	1.00	36.64
ATOM	4711	C	ALA	615	63.942	5.838	31.202	1.00	35.36
ATOM	4712	O	ALA	615	64.065	6.805	31.952	1.00	36.80
ATOM	4713	N	SER	616	64.690	4.739	31.315	1.00	35.91
ATOM	4715	CA	SER	616	65.716	4.621	32.354	1.00	35.78
ATOM	4716	CB	SER	616	66.287	3.199	32.424	1.00	32.52
ATOM	4717	OG	SER	616	67.133	2.899	31.324	1.00	29.64
ATOM	4719	C	SER	616	66.832	5.623	32.063	1.00	37.48
ATOM	4720	O	SER	616	67.556	6.048	32.967	1.00	38.76
ATOM	4721	N	LYS	617	66.971	5.980	30.790	1.00	34.74
ATOM	4723	CA	LYS	617	67.973	6.931	30.357	1.00	32.44
ATOM	4724	CB	LYS	617	68.540	6.520	28.998	1.00	32.94
ATOM	4725	CG	LYS	617	69.330	5.232	29.041	1.00	32.64
ATOM	4726	CD	LYS	617	70.539	5.402	29.933	1.00	38.45
ATOM	4727	CE	LYS	617	71.252	4.091	30.139	1.00	40.84
ATOM	4728	NZ	LYS	617	72.552	4.306	30.812	1.00	46.49
ATOM	4732	C	LYS	617	67.376	8.325	30.281	1.00	33.29
ATOM	4733	O	LYS	617	67.909	9.188	29.598	1.00	33.95
ATOM	4734	N	LYS	618	66.245	8.528	30.952	1.00	34.87
ATOM	4736	CA	LYS	618	65.569	9.822	30.997	1.00	35.44
ATOM	4737	CB	LYS	618	66.512	10.868	31.581	1.00	40.44
ATOM	4738	CG	LYS	618	67.192	10.446	32.877	1.00	48.19
ATOM	4739	CD	LYS	618	66.234	10.363	34.037	1.00	55.47
ATOM	4740	CE	LYS	618	66.962	9.939	35.310	1.00	61.56
ATOM	4741	NZ	LYS	618	66.070	10.032	36.514	1.00	68.82
ATOM	4745	C	LYS	618	65.015	10.327	29.663	1.00	35.62
ATOM	4746	O	LYS	618	64.557	11.463	29.569	1.00	36.44
ATOM	4747	N	CYS	619	65.006	9.472	28.647	1.00	34.24
ATOM	4749	CA	CYS	619	64.525	9.848	27.323	1.00	31.62

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ATOM	4750	CB	CYS	619	65.279	9.033	26.263	1.00	31.17
ATOM	4751	SG	CYS	619	64.816	9.306	24.541	1.00	30.02
ATOM	4752	C	CYS	619	63.004	9.701	27.149	1.00	30.45
ATOM	4753	O	CYS	619	62.418	8.649	27.388	1.00	29.24
ATOM	4754	N	ILE	620	62.359	10.798	26.800	1.00	30.14
ATOM	4756	CA	ILE	620	60.935	10.822	26.542	1.00	31.76
ATOM	4757	CB	ILE	620	60.268	12.040	27.193	1.00	31.26
ATOM	4758	CG2	ILE	620	58.799	12.116	26.774	1.00	31.66
ATOM	4759	CG1	ILE	620	60.392	11.957	28.712	1.00	29.71
ATOM	4760	CD1	ILE	620	60.016	13.236	29.396	1.00	27.40
ATOM	4761	C	ILE	620	60.864	10.961	25.023	1.00	31.86
ATOM	4762	O	ILE	620	61.384	11.920	24.465	1.00	32.70
ATOM	4763	N	HIS	621	60.249	9.986	24.366	1.00	31.70
ATOM	4765	CA	HIS	621	60.133	9.973	22.906	1.00	32.12
ATOM	4766	CB	HIS	621	59.708	8.578	22.430	1.00	29.61
ATOM	4767	CG	HIS	621	59.903	8.344	20.961	1.00	28.62
ATOM	4768	CD2	HIS	621	60.511	7.336	20.300	1.00	27.49
ATOM	4769	ND1	HIS	621	59.373	9.168	19.988	1.00	30.08
ATOM	4771	CE1	HIS	621	59.637	8.669	18.795	1.00	25.00
ATOM	4772	NE2	HIS	621	60.325	7.554	18.956	1.00	26.55
ATOM	4774	C	HIS	621	59.194	11.026	22.321	1.00	34.51
ATOM	4775	O	HIS	621	59.466	11.570	21.251	1.00	36.79
ATOM	4776	N	ARG	622	58.048	11.248	22.960	1.00	35.26
ATOM	4778	CA	ARG	622	57.068	12.239	22.490	1.00	34.68
ATOM	4779	CB	ARG	622	57.705	13.628	22.370	1.00	33.43
ATOM	4780	CG	ARG	622	58.285	14.135	23.674	1.00	31.52
ATOM	4781	CD	ARG	622	58.781	15.563	23.570	0.50	27.82
ATOM	4782	NE	ARG	622	59.216	16.050	24.876	0.50	28.82
ATOM	4784	CZ	ARG	622	60.362	15.715	25.463	0.50	30.41
ATOM	4785	NH1	ARG	622	61.215	14.891	24.860	0.50	31.15
ATOM	4788	NH2	ARG	622	60.640	16.168	26.680	0.50	30.83
ATOM	4791	C	ARG	622	56.283	11.891	21.213	1.00	34.71
ATOM	4792	O	ARG	622	55.289	12.544	20.912	1.00	35.58
ATOM	4793	N	ASP	623	56.719	10.884	20.459	1.00	34.90
ATOM	4795	CA	ASP	623	55.986	10.468	19.261	1.00	34.30
ATOM	4796	CB	ASP	623	56.443	11.212	17.994	1.00	36.76
ATOM	4797	CG	ASP	623	55.535	10.918	16.772	1.00	43.35
ATOM	4798	OD1	ASP	623	55.980	11.131	15.624	1.00	47.64
ATOM	4799	OD2	ASP	623	54.376	10.469	16.954	1.00	43.30
ATOM	4800	C	ASP	623	56.094	8.967	19.051	1.00	32.24
ATOM	4801	O	ASP	623	56.406	8.494	17.957	1.00	31.19
ATOM	4802	N	LEU	624	55.895	8.209	20.118	1.00	32.27
ATOM	4804	CA	LEU	624	55.964	6.759	20.005	1.00	33.18
ATOM	4805	CB	LEU	624	56.013	6.118	21.390	1.00	31.16
ATOM	4806	CG	LEU	624	56.019	4.592	21.452	1.00	32.74
ATOM	4807	CD1	LEU	624	57.257	4.020	20.765	1.00	30.64
ATOM	4808	CD2	LEU	624	55.974	4.177	22.904	1.00	34.51
ATOM	4809	C	LEU	624	54.738	6.274	19.217	1.00	35.18
ATOM	4810	O	LEU	624	53.589	6.511	19.612	1.00	35.72
ATOM	4811	N	ALA	625	54.997	5.632	18.084	1.00	32.37
ATOM	4813	CA	ALA	625	53.946	5.113	17.223	1.00	30.60
ATOM	4814	CB	ALA	625	53.447	6.205	16.298	1.00	25.26
ATOM	4815	C	ALA	625	54.618	4.020	16.427	1.00	29.87
ATOM	4816	O	ALA	625	55.839	3.978	16.378	1.00	32.01

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ATOM	4817	N	ALA	626	53.834	3.163	15.779	1.00	30.12
ATOM	4819	CA	ALA	626	54.373	2.057	14.978	1.00	29.62
ATOM	4820	CB	ALA	626	53.231	1.159	14.441	1.00	27.11
ATOM	4821	C	ALA	626	55.255	2.552	13.838	1.00	26.57
ATOM	4822	O	ALA	626	56.193	1.871	13.434	1.00	26.29
ATOM	4823	N	ARG	627	54.935	3.730	13.317	1.00	26.74
ATOM	4825	CA	ARG	627	55.706	4.352	12.244	1.00	28.73
ATOM	4826	CB	ARG	627	55.056	5.671	11.827	1.00	29.62
ATOM	4827	CG	ARG	627	54.894	6.659	12.972	1.00	31.84
ATOM	4828	CD	ARG	627	54.435	8.032	12.485	1.00	38.54
ATOM	4829	NE	ARG	627	53.987	8.878	13.590	1.00	38.59
ATOM	4831	CZ	ARG	627	52.745	8.879	14.064	1.00	39.55
ATOM	4832	NH1	ARG	627	51.822	8.094	13.525	1.00	35.96
ATOM	4835	NH2	ARG	627	52.447	9.604	15.127	1.00	41.05
ATOM	4838	C	ARG	627	57.151	4.632	12.676	1.00	30.79
ATOM	4839	O	ARG	627	58.058	4.687	11.838	1.00	30.16
ATOM	4840	N	ASN	628	57.347	4.822	13.985	1.00	30.31
ATOM	4842	CA	ASN	628	58.661	5.109	14.550	1.00	28.50
ATOM	4843	CB	ASN	628	58.587	6.257	15.549	1.00	27.84
ATOM	4844	CG	ASN	628	58.369	7.571	14.868	1.00	31.41
ATOM	4845	OD1	ASN	628	58.893	7.796	13.782	1.00	33.45
ATOM	4846	ND2	ASN	628	57.551	8.429	15.460	1.00	28.53
ATOM	4849	C	ASN	628	59.352	3.919	15.169	1.00	28.10
ATOM	4850	O	ASN	628	60.232	4.076	16.021	1.00	28.64
ATOM	4851	N	VAL	629	58.887	2.733	14.803	1.00	27.79
ATOM	4853	CA	VAL	629	59.484	1.482	15.253	1.00	28.30
ATOM	4854	CB	VAL	629	58.475	0.577	15.983	1.00	25.38
ATOM	4855	CG1	VAL	629	59.118	-0.753	16.284	1.00	23.07
ATOM	4856	CG2	VAL	629	57.980	1.246	17.265	1.00	22.48
ATOM	4857	C	VAL	629	59.925	0.810	13.949	1.00	28.69
ATOM	4858	O	VAL	629	59.114	0.616	13.043	1.00	27.07
ATOM	4859	N	LEU	630	61.220	0.542	13.823	1.00	29.54
ATOM	4861	CA	LEU	630	61.749	-0.081	12.616	1.00	30.17
ATOM	4862	CB	LEU	630	62.999	0.659	12.142	1.00	29.62
ATOM	4863	CG	LEU	630	62.831	2.180	12.035	1.00	29.14
ATOM	4864	CD1	LEU	630	64.121	2.795	11.579	1.00	29.83
ATOM	4865	CD2	LEU	630	61.693	2.543	11.086	1.00	32.59
ATOM	4866	C	LEU	630	62.036	-1.541	12.899	1.00	30.50
ATOM	4867	O	LEU	630	62.290	-1.910	14.042	1.00	31.06
ATOM	4868	N	VAL	631	61.966	-2.376	11.866	1.00	33.03
ATOM	4870	CA	VAL	631	62.174	-3.813	12.022	1.00	31.83
ATOM	4871	CB	VAL	631	60.902	-4.605	11.582	1.00	29.48
ATOM	4872	CG1	VAL	631	61.017	-6.067	11.980	1.00	29.39
ATOM	4873	CG2	VAL	631	59.644	-3.984	12.196	1.00	25.38
ATOM	4874	C	VAL	631	63.379	-4.242	11.196	1.00	32.37
ATOM	4875	O	VAL	631	63.508	-3.865	10.024	1.00	33.57
ATOM	4876	N	THR	632	64.285	-4.987	11.820	1.00	34.39
ATOM	4878	CA	THR	632	65.504	-5.453	11.145	1.00	35.84
ATOM	4879	CB	THR	632	66.659	-5.685	12.148	1.00	33.11
ATOM	4880	OG1	THR	632	66.328	-6.774	13.020	1.00	34.88
ATOM	4882	CG2	THR	632	66.922	-4.426	12.972	1.00	28.85
ATOM	4883	C	THR	632	65.272	-6.738	10.350	1.00	37.63
ATOM	4884	O	THR	632	64.195	-7.347	10.439	1.00	37.20
ATOM	4885	N	GLU	633	66.289	-7.163	9.600	1.00	39.78

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ATOM	4887	CA	GLU	633	66.182	-8.379	8.794	1.00	43.30
ATOM	4888	CB	GLU	633	67.437	-8.590	7.933	1.00	46.66
ATOM	4889	CG	GLU	633	67.336	-9.729	6.876	1.00	51.37
ATOM	4890	CD	GLU	633	66.490	-9.404	5.622	1.00	54.30
ATOM	4891	OE1	GLU	633	65.859	-8.327	5.523	1.00	55.85
ATOM	4892	OE2	GLU	633	66.460	-10.256	4.710	1.00	55.95
ATOM	4893	C	GLU	633	65.919	-9.592	9.677	1.00	42.72
ATOM	4894	O	GLU	633	65.360	-10.582	9.222	1.00	45.10
ATOM	4895	N	ASP	634	66.287	-9.494	10.949	1.00	42.83
ATOM	4897	CA	ASP	634	66.075	-10.585	11.884	1.00	43.03
ATOM	4898	CB	ASP	634	67.324	-10.809	12.743	1.00	49.02
ATOM	4899	CG	ASP	634	68.539	-11.240	11.916	1.00	55.95
ATOM	4900	OD1	ASP	634	68.462	-12.292	11.237	1.00	59.10
ATOM	4901	OD2	ASP	634	69.568	-10.525	11.943	1.00	59.41
ATOM	4902	C	ASP	634	64.848	-10.340	12.751	1.00	41.75
ATOM	4903	O	ASP	634	64.737	-10.873	13.847	1.00	42.79
ATOM	4904	N	ASN	635	63.937	-9.508	12.257	1.00	42.51
ATOM	4906	CA	ASN	635	62.686	-9.186	12.939	1.00	42.53
ATOM	4907	CB	ASN	635	61.768	-10.417	12.992	1.00	45.07
ATOM	4908	CG	ASN	635	61.483	-10.985	11.624	1.00	46.54
ATOM	4909	OD1	ASN	635	60.868	-10.336	10.786	1.00	49.77
ATOM	4910	ND2	ASN	635	61.949	-12.192	11.383	1.00	49.29
ATOM	4913	C	ASN	635	62.801	-8.577	14.331	1.00	40.51
ATOM	4914	O	ASN	635	61.939	-8.800	15.187	1.00	41.80
ATOM	4915	N	VAL	636	63.844	-7.795	14.561	1.00	37.98
ATOM	4917	CA	VAL	636	64.016	-7.164	15.856	1.00	33.92
ATOM	4918	CB	VAL	636	65.517	-7.005	16.195	1.00	32.21
ATOM	4919	CG1	VAL	636	65.697	-6.284	17.530	1.00	31.40
ATOM	4920	CG2	VAL	636	66.169	-8.367	16.242	1.00	30.93
ATOM	4921	C	VAL	636	63.349	-5.797	15.811	1.00	31.85
ATOM	4922	O	VAL	636	63.531	-5.061	14.849	1.00	33.47
ATOM	4923	N	MET	637	62.525	-5.492	16.807	1.00	31.69
ATOM	4925	CA	MET	637	61.860	-4.194	16.879	1.00	31.44
ATOM	4926	CB	MET	637	60.642	-4.241	17.820	1.00	34.97
ATOM	4927	CG	MET	637	59.559	-5.264	17.455	1.00	36.80
ATOM	4928	SD	MET	637	58.860	-5.048	15.803	1.00	35.45
ATOM	4929	CE	MET	637	59.030	-6.709	15.116	1.00	32.12
ATOM	4930	C	MET	637	62.874	-3.209	17.454	1.00	31.86
ATOM	4931	O	MET	637	63.512	-3.496	18.479	1.00	29.47
ATOM	4932	N	LYS	638	62.985	-2.041	16.820	1.00	30.87
ATOM	4934	CA	LYS	638	63.915	-0.994	17.244	1.00	29.66
ATOM	4935	CB	LYS	638	65.161	-0.983	16.349	1.00	27.51
ATOM	4936	CG	LYS	638	66.171	-2.059	16.691	1.00	27.29
ATOM	4937	CD	LYS	638	67.370	-1.984	15.781	1.00	28.55
ATOM	4938	CE	LYS	638	68.409	-3.029	16.150	1.00	24.75
ATOM	4939	NZ	LYS	638	68.964	-2.785	17.498	1.00	25.59
ATOM	4943	C	LYS	638	63.283	0.383	17.215	1.00	27.72
ATOM	4944	O	LYS	638	62.918	0.869	16.146	1.00	27.66
ATOM	4945	N	ILE	639	63.163	1.004	18.387	1.00	26.21
ATOM	4947	CA	ILE	639	62.597	2.343	18.501	1.00	26.27
ATOM	4948	CB	ILE	639	62.580	2.862	19.965	1.00	26.52
ATOM	4949	CG2	ILE	639	61.896	4.206	20.017	1.00	21.50
ATOM	4950	CG1	ILE	639	61.918	1.854	20.926	1.00	25.70
ATOM	4951	CD1	ILE	639	60.496	1.494	20.599	1.00	25.62

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ATOM	4952	C	ILE	639	63.505	3.288	17.718	1.00	29.56
ATOM	4953	O	ILE	639	64.730	3.281	17.906	1.00	27.74
ATOM	4954	N	ALA	640	62.897	4.101	16.857	1.00	27.91
ATOM	4956	CA	ALA	640	63.620	5.071	16.042	1.00	28.79
ATOM	4957	CB	ALA	640	63.377	4.796	14.563	1.00	26.74
ATOM	4958	C	ALA	640	63.164	6.487	16.385	1.00	28.91
ATOM	4959	O	ALA	640	62.087	6.683	16.956	1.00	28.67
ATOM	4960	N	ASP	641	64.007	7.464	16.067	1.00	28.25
ATOM	4962	CA	ASP	641	63.708	8.876	16.296	1.00	30.80
ATOM	4963	CB	ASP	641	62.520	9.319	15.428	1.00	33.44
ATOM	4964	CG	ASP	641	62.869	9.393	13.948	1.00	38.01
ATOM	4965	OD1	ASP	641	64.002	9.001	13.574	1.00	42.41
ATOM	4966	OD2	ASP	641	62.006	9.847	13.160	1.00	41.74
ATOM	4967	C	ASP	641	63.501	9.311	17.745	1.00	29.07
ATOM	4968	O	ASP	641	62.847	10.309	18.020	1.00	28.42
ATOM	4969	N	PHE	642	64.138	8.604	18.663	1.00	29.69
ATOM	4971	CA	PHE	642	64.036	8.914	20.074	1.00	29.62
ATOM	4972	CB	PHE	642	64.347	7.656	20.890	1.00	27.18
ATOM	4973	CG	PHE	642	65.702	7.058	20.603	1.00	23.96
ATOM	4974	CD1	PHE	642	66.848	7.559	21.219	1.00	23.66
ATOM	4975	CD2	PHE	642	65.828	5.974	19.742	1.00	24.08
ATOM	4976	CE1	PHE	642	68.090	6.992	20.980	1.00	23.02
ATOM	4977	CE2	PHE	642	67.069	5.403	19.501	1.00	23.20
ATOM	4978	CZ	PHE	642	68.200	5.909	20.121	1.00	21.68
ATOM	4979	C	PHE	642	64.948	10.075	20.502	1.00	32.99
ATOM	4980	O	PHE	642	64.755	10.664	21.574	1.00	32.10
ATOM	4981	N	GLY	643	65.940	10.396	19.671	1.00	34.66
ATOM	4983	CA	GLY	643	66.869	11.463	20.003	1.00	35.29
ATOM	4984	C	GLY	643	66.639	12.755	19.250	1.00	39.13
ATOM	4985	O	GLY	643	67.464	13.666	19.333	1.00	39.83
ATOM	4986	N	LEU	644	65.520	12.850	18.532	1.00	42.26
ATOM	4988	CA	LEU	644	65.202	14.043	17.745	1.00	46.25
ATOM	4989	CB	LEU	644	63.935	13.843	16.911	1.00	44.59
ATOM	4990	CG	LEU	644	63.911	12.839	15.763	1.00	43.00
ATOM	4991	CD1	LEU	644	62.653	13.068	14.940	1.00	42.61
ATOM	4992	CD2	LEU	644	65.119	13.016	14.889	1.00	45.65
ATOM	4993	C	LEU	644	65.037	15.298	18.578	1.00	49.59
ATOM	4994	O	LEU	644	64.391	15.281	19.623	1.00	51.90
ATOM	4995	N	ALA	645	65.585	16.401	18.080	1.00	52.08
ATOM	4997	CA	ALA	645	65.495	17.677	18.777	1.00	54.71
ATOM	4998	CB	ALA	645	66.414	18.699	18.124	1.00	54.38
ATOM	4999	C	ALA	645	64.053	18.184	18.790	1.00	55.44
ATOM	5000	O	ALA	645	63.534	18.582	19.832	1.00	56.69
ATOM	5001	N	ASP	652	52.389	21.543	14.759	1.00	73.74
ATOM	5003	CA	ASP	652	51.207	21.745	13.934	1.00	73.83
ATOM	5004	CB	ASP	652	51.601	21.995	12.472	1.00	73.22
ATOM	5005	CG	ASP	652	50.398	22.241	11.569	1.00	72.95
ATOM	5006	OD1	ASP	652	49.354	22.715	12.065	1.00	73.71
ATOM	5007	OD2	ASP	652	50.497	21.956	10.357	1.00	73.02
ATOM	5008	C	ASP	652	50.321	20.514	14.042	1.00	75.11
ATOM	5009	O	ASP	652	50.568	19.495	13.394	1.00	75.96
ATOM	5010	N	TYR	653	49.272	20.628	14.849	1.00	75.57
ATOM	5012	CA	TYR	653	48.348	19.524	15.064	1.00	75.68
ATOM	5013	CB	TYR	653	47.274	19.914	16.088	1.00	76.85

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ATOM	5014	CG	TYR	653	47.771	19.995	17.519	1.00	79.55
ATOM	5015	CD1	TYR	653	46.983	20.567	18.518	1.00	80.89
ATOM	5016	CE1	TYR	653	47.438	20.648	19.836	1.00	83.02
ATOM	5017	CD2	TYR	653	49.032	19.503	17.874	1.00	80.87
ATOM	5018	CE2	TYR	653	49.496	19.578	19.183	1.00	81.70
ATOM	5019	CZ	TYR	653	48.698	20.152	20.160	1.00	83.09
ATOM	5020	OH	TYR	653	49.165	20.243	21.451	1.00	83.73
ATOM	5022	C	TYR	653	47.685	19.038	13.787	1.00	75.03
ATOM	5023	O	TYR	653	47.232	17.897	13.711	1.00	75.97
ATOM	5024	N	TYR	654	47.679	19.885	12.767	1.00	73.85
ATOM	5026	CA	TYR	654	47.039	19.538	11.507	1.00	73.32
ATOM	5027	CB	TYR	654	46.276	20.750	10.972	1.00	71.97
ATOM	5028	CG	TYR	654	45.259	21.276	11.954	1.00	70.94
ATOM	5029	CD1	TYR	654	45.659	21.801	13.185	1.00	71.41
ATOM	5030	CE1	TYR	654	44.733	22.234	14.121	1.00	73.60
ATOM	5031	CD2	TYR	654	43.899	21.206	11.680	1.00	71.81
ATOM	5032	CE2	TYR	654	42.956	21.642	12.610	1.00	74.81
ATOM	5033	CZ	TYR	654	43.380	22.152	13.832	1.00	74.84
ATOM	5034	OH	TYR	654	42.457	22.571	14.769	1.00	76.60
ATOM	5036	C	TYR	654	47.975	18.967	10.446	1.00	73.82
ATOM	5037	O	TYR	654	47.545	18.671	9.329	1.00	74.25
ATOM	5038	N	LYS	655	49.249	18.806	10.784	1.00	74.04
ATOM	5040	CA	LYS	655	50.195	18.256	9.827	1.00	75.41
ATOM	5041	CB	LYS	655	51.626	18.680	10.164	1.00	78.45
ATOM	5042	CG	LYS	655	52.647	18.198	9.151	1.00	83.01
ATOM	5043	CD	LYS	655	54.062	18.589	9.537	1.00	87.72
ATOM	5044	CE	LYS	655	55.076	17.813	8.703	1.00	91.45
ATOM	5045	NZ	LYS	655	56.489	18.133	9.074	1.00	94.17
ATOM	5049	C	LYS	655	50.075	16.736	9.832	1.00	75.50
ATOM	5050	O	LYS	655	50.245	16.092	10.872	1.00	75.90
ATOM	5051	N	LYS	656	49.750	16.173	8.672	1.00	75.26
ATOM	5053	CA	LYS	656	49.597	14.730	8.533	1.00	74.97
ATOM	5054	CB	LYS	656	48.723	14.406	7.323	1.00	75.40
ATOM	5055	CG	LYS	656	47.266	14.753	7.519	1.00	76.87
ATOM	5056	CD	LYS	656	46.489	14.535	6.239	1.00	80.75
ATOM	5057	CE	LYS	656	45.001	14.655	6.483	1.00	83.60
ATOM	5058	NZ	LYS	656	44.236	14.637	5.204	1.00	87.14
ATOM	5062	C	LYS	656	50.939	14.016	8.414	1.00	74.58
ATOM	5063	O	LYS	656	51.904	14.578	7.897	1.00	75.01
ATOM	5064	N	GLY	660	49.137	9.764	5.736	1.00	59.18
ATOM	5066	CA	GLY	660	48.106	10.781	5.848	1.00	56.19
ATOM	5067	C	GLY	660	47.407	10.761	7.192	1.00	55.31
ATOM	5068	O	GLY	660	46.289	11.263	7.328	1.00	56.96
ATOM	5069	N	ARG	661	48.059	10.163	8.183	1.00	53.02
ATOM	5071	CA	ARG	661	47.493	10.083	9.527	1.00	49.80
ATOM	5072	CB	ARG	661	47.944	8.799	10.229	1.00	51.79
ATOM	5073	CG	ARG	661	47.683	7.523	9.450	1.00	50.59
ATOM	5074	CD	ARG	661	47.822	6.323	10.367	1.00	53.68
ATOM	5075	NE	ARG	661	47.714	5.044	9.665	1.00	52.66
ATOM	5077	CZ	ARG	661	47.928	3.863	10.236	1.00	51.73
ATOM	5078	NH1	ARG	661	48.264	3.794	11.518	1.00	50.23
ATOM	5081	NH2	ARG	661	47.800	2.751	9.528	1.00	52.58
ATOM	5084	C	ARG	661	47.915	11.297	10.346	1.00	44.80
ATOM	5085	O	ARG	661	48.865	11.998	9.986	1.00	43.61

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ATOM	5086	N	LEU	662	47.221	11.528	11.453	1.00	40.74
ATOM	5088	CA	LEU	662	47.518	12.654	12.333	1.00	37.88
ATOM	5089	CB	LEU	662	46.234	13.415	12.671	1.00	36.19
ATOM	5090	CG	LEU	662	45.515	14.074	11.499	1.00	35.32
ATOM	5091	CD1	LEU	662	44.045	14.278	11.831	1.00	31.05
ATOM	5092	CD2	LEU	662	46.217	15.383	11.156	1.00	34.37
ATOM	5093	C	LEU	662	48.162	12.170	13.622	1.00	35.34
ATOM	5094	O	LEU	662	47.529	11.479	14.417	1.00	33.06
ATOM	5095	N	PRO	663	49.441	12.518	13.843	1.00	36.39
ATOM	5096	CD	PRO	663	50.375	13.113	12.868	1.00	37.57
ATOM	5097	CA	PRO	663	50.158	12.107	15.054	1.00	36.39
ATOM	5098	CB	PRO	663	51.516	12.787	14.885	1.00	36.98
ATOM	5099	CG	PRO	663	51.728	12.657	13.401	1.00	38.48
ATOM	5100	C	PRO	663	49.477	12.491	16.371	1.00	35.47
ATOM	5101	O	PRO	663	49.699	11.841	17.392	1.00	35.08
ATOM	5102	N	VAL	664	48.646	13.532	16.362	1.00	34.28
ATOM	5104	CA	VAL	664	47.951	13.931	17.583	1.00	34.43
ATOM	5105	CB	VAL	664	47.038	15.181	17.376	1.00	36.92
ATOM	5106	CG1	VAL	664	47.885	16.408	17.160	1.00	37.55
ATOM	5107	CG2	VAL	664	46.091	14.989	16.186	1.00	38.28
ATOM	5108	C	VAL	664	47.137	12.749	18.120	1.00	33.03
ATOM	5109	O	VAL	664	46.908	12.641	19.318	1.00	34.62
ATOM	5110	N	LYS	665	46.803	11.809	17.236	1.00	32.47
ATOM	5112	CA	LYS	665	46.040	10.631	17.614	1.00	30.71
ATOM	5113	CB	LYS	665	45.456	9.958	16.370	1.00	29.59
ATOM	5114	CG	LYS	665	44.324	10.774	15.768	1.00	29.64
ATOM	5115	CD	LYS	665	43.927	10.334	14.367	1.00	31.86
ATOM	5116	CE	LYS	665	42.664	11.056	13.899	1.00	30.42
ATOM	5117	NZ	LYS	665	42.296	10.720	12.486	1.00	26.50
ATOM	5121	C	LYS	665	46.801	9.644	18.498	1.00	32.23
ATOM	5122	O	LYS	665	46.230	8.659	18.955	1.00	30.04
ATOM	5123	N	TRP	666	48.080	9.915	18.748	1.00	31.38
ATOM	5125	CA	TRP	666	48.886	9.068	19.619	1.00	32.32
ATOM	5126	CB	TRP	666	50.204	8.682	18.945	1.00	31.07
ATOM	5127	CG	TRP	666	50.078	7.530	18.006	1.00	28.26
ATOM	5128	CD2	TRP	666	49.531	7.559	16.684	1.00	27.07
ATOM	5129	CE2	TRP	666	49.630	6.257	16.163	1.00	26.71
ATOM	5130	CE3	TRP	666	48.982	8.569	15.882	1.00	26.56
ATOM	5131	CD1	TRP	666	50.473	6.238	18.234	1.00	24.97
ATOM	5132	NE1	TRP	666	50.206	5.469	17.132	1.00	27.38
ATOM	5134	CZ2	TRP	666	49.190	5.929	14.874	1.00	27.22
ATOM	5135	CZ3	TRP	666	48.548	8.248	14.599	1.00	30.14
ATOM	5136	CH2	TRP	666	48.658	6.934	14.107	1.00	26.64
ATOM	5137	C	TRP	666	49.203	9.802	20.913	1.00	33.84
ATOM	5138	O	TRP	666	49.688	9.202	21.873	1.00	32.82
ATOM	5139	N	MET	667	48.905	11.099	20.929	1.00	35.75
ATOM	5141	CA	MET	667	49.180	11.960	22.069	1.00	37.60
ATOM	5142	CB	MET	667	49.150	13.423	21.641	1.00	41.95
ATOM	5143	CG	MET	667	50.487	13.975	21.226	1.00	48.44
ATOM	5144	SD	MET	667	50.384	15.728	20.919	1.00	55.33
ATOM	5145	CE	MET	667	50.711	15.745	19.183	1.00	49.29
ATOM	5146	C	MET	667	48.294	11.802	23.289	1.00	38.98
ATOM	5147	O	MET	667	47.066	11.699	23.183	1.00	39.18
ATOM	5148	N	ALA	668	48.933	11.824	24.456	1.00	38.72

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ATOM	5150	CA	ALA	668	48.231	11.728	25.727	1.00	37.82
ATOM	5151	CB	ALA	668	49.224	11.527	26.857	1.00	38.49
ATOM	5152	C	ALA	668	47.497	13.051	25.891	1.00	38.16
ATOM	5153	O	ALA	668	47.937	14.072	25.363	1.00	37.21
ATOM	5154	N	PRO	669	46.383	13.062	26.644	1.00	39.78
ATOM	5155	CD	PRO	669	45.785	11.931	27.367	1.00	40.08
ATOM	5156	CA	PRO	669	45.598	14.281	26.858	1.00	40.68
ATOM	5157	CB	PRO	669	44.474	13.806	27.782	1.00	42.15
ATOM	5158	CG	PRO	669	44.346	12.352	27.446	1.00	42.56
ATOM	5159	C	PRO	669	46.398	15.432	27.484	1.00	42.69
ATOM	5160	O	PRO	669	46.320	16.566	27.019	1.00	42.14
ATOM	5161	N	GLU	670	47.168	15.153	28.532	1.00	43.21
ATOM	5163	CA	GLU	670	47.956	16.211	29.160	1.00	44.62
ATOM	5164	CB	GLU	670	48.651	15.719	30.429	1.00	44.95
ATOM	5165	CG	GLU	670	49.824	14.782	30.197	1.00	45.54
ATOM	5166	CD	GLU	670	49.422	13.332	30.079	1.00	42.72
ATOM	5167	OE1	GLU	670	50.332	12.481	30.066	1.00	41.43
ATOM	5168	OE2	GLU	670	48.212	13.036	30.015	1.00	44.44
ATOM	5169	C	GLU	670	48.993	16.772	28.195	1.00	44.88
ATOM	5170	O	GLU	670	49.248	17.968	28.194	1.00	45.08
ATOM	5171	N	ALA	671	49.565	15.908	27.358	1.00	44.75
ATOM	5173	CA	ALA	671	50.573	16.323	26.392	1.00	45.92
ATOM	5174	CB	ALA	671	51.256	15.095	25.766	1.00	44.10
ATOM	5175	C	ALA	671	49.944	17.193	25.314	1.00	47.96
ATOM	5176	O	ALA	671	50.526	18.192	24.894	1.00	49.16
ATOM	5177	N	LEU	672	48.729	16.836	24.917	1.00	49.84
ATOM	5179	CA	LEU	672	47.989	17.554	23.881	1.00	50.74
ATOM	5180	CB	LEU	672	46.926	16.619	23.289	1.00	53.20
ATOM	5181	CG	LEU	672	46.184	16.989	22.004	1.00	55.26
ATOM	5182	CD1	LEU	672	47.153	17.155	20.856	1.00	57.12
ATOM	5183	CD2	LEU	672	45.203	15.895	21.680	1.00	52.86
ATOM	5184	C	LEU	672	47.327	18.826	24.408	1.00	50.79
ATOM	5185	O	LEU	672	47.302	19.855	23.736	1.00	50.95
ATOM	5186	N	PHE	673	46.792	18.751	25.618	1.00	52.07
ATOM	5188	CA	PHE	673	46.111	19.884	26.226	1.00	54.39
ATOM	5189	CB	PHE	673	44.892	19.396	27.019	1.00	51.21
ATOM	5190	CG	PHE	673	43.871	18.656	26.186	1.00	48.49
ATOM	5191	CD1	PHE	673	43.304	17.473	26.646	1.00	47.79
ATOM	5192	CD2	PHE	673	43.470	19.149	24.949	1.00	49.04
ATOM	5193	CE1	PHE	673	42.349	16.789	25.888	1.00	47.90
ATOM	5194	CE2	PHE	673	42.511	18.473	24.182	1.00	49.71
ATOM	5195	CZ	PHE	673	41.952	17.288	24.655	1.00	46.86
ATOM	5196	C	PHE	673	47.007	20.741	27.123	1.00	58.25
ATOM	5197	O	PHE	673	47.000	21.971	27.034	1.00	60.52
ATOM	5198	N	ASP	674	47.784	20.094	27.983	1.00	59.63
ATOM	5200	CA	ASP	674	48.652	20.815	28.905	1.00	62.11
ATOM	5201	CB	ASP	674	48.568	20.196	30.307	1.00	63.81
ATOM	5202	CG	ASP	674	47.143	20.015	30.791	1.00	66.46
ATOM	5203	OD1	ASP	674	46.815	18.901	31.247	1.00	66.70
ATOM	5204	OD2	ASP	674	46.354	20.981	30.722	1.00	68.77
ATOM	5205	C	ASP	674	50.119	20.852	28.482	1.00	63.36
ATOM	5206	O	ASP	674	50.979	21.175	29.310	1.00	64.11
ATOM	5207	N	ARG	675	50.410	20.486	27.228	1.00	62.94
ATOM	5209	CA	ARG	675	51.789	20.456	26.706	1.00	60.75

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ATOM	5210	CB	ARG	675	52.277	21.874	26.360	1.00	60.56
ATOM	5211	CG	ARG	675	51.474	22.560	25.261	1.00	63.67
ATOM	5212	CD	ARG	675	51.986	23.970	24.964	1.00	66.99
ATOM	5213	NE	ARG	675	53.308	23.980	24.337	1.00	69.34
ATOM	5215	CZ	ARG	675	54.063	25.068	24.173	1.00	68.48
ATOM	5216	NH1	ARG	675	53.637	26.254	24.590	1.00	65.81
ATOM	5219	NH2	ARG	675	55.254	24.965	23.593	1.00	68.76
ATOM	5222	C	ARG	675	52.750	19.793	27.700	1.00	58.06
ATOM	5223	O	ARG	675	53.933	20.130	27.766	1.00	59.30
ATOM	5224	N	ILE	676	52.221	18.859	28.483	1.00	55.62
ATOM	5226	CA	ILE	676	52.992	18.141	29.489	1.00	54.09
ATOM	5227	CB	ILE	676	52.154	17.921	30.765	1.00	52.69
ATOM	5228	CG2	ILE	676	52.749	16.811	31.629	1.00	49.38
ATOM	5229	CG1	ILE	676	52.049	19.230	31.540	1.00	53.15
ATOM	5230	CD1	ILE	676	51.306	19.103	32.845	1.00	57.79
ATOM	5231	C	ILE	676	53.468	16.796	28.953	1.00	53.83
ATOM	5232	O	ILE	676	52.668	15.891	28.730	1.00	54.87
ATOM	5233	N	TYR	677	54.773	16.671	28.745	1.00	51.76
ATOM	5235	CA	TYR	677	55.343	15.436	28.236	1.00	49.42
ATOM	5236	CB	TYR	677	56.232	15.722	27.031	1.00	51.33
ATOM	5237	CG	TYR	677	55.466	16.181	25.809	1.00	56.22
ATOM	5238	CD1	TYR	677	55.158	17.529	25.619	1.00	56.12
ATOM	5239	CE1	TYR	677	54.491	17.960	24.479	1.00	56.18
ATOM	5240	CD2	TYR	677	55.078	15.269	24.823	1.00	58.13
ATOM	5241	CE2	TYR	677	54.411	15.689	23.679	1.00	57.65
ATOM	5242	CZ	TYR	677	54.125	17.035	23.512	1.00	58.23
ATOM	5243	OH	TYR	677	53.504	17.457	22.360	1.00	61.71
ATOM	5245	C	TYR	677	56.136	14.730	29.316	1.00	46.46
ATOM	5246	O	TYR	677	56.983	15.335	29.970	1.00	48.65
ATOM	5247	N	THR	678	55.818	13.464	29.537	1.00	41.73
ATOM	5249	CA	THR	678	56.498	12.664	30.535	1.00	39.83
ATOM	5250	CB	THR	678	55.680	12.593	31.861	1.00	41.78
ATOM	5251	OG1	THR	678	54.462	11.867	31.642	1.00	45.77
ATOM	5253	CG2	THR	678	55.342	13.988	32.383	1.00	41.84
ATOM	5254	C	THR	678	56.661	11.242	30.011	1.00	37.46
ATOM	5255	O	THR	678	56.258	10.917	28.897	1.00	37.51
ATOM	5256	N	HIS	679	57.264	10.388	30.825	1.00	36.36
ATOM	5258	CA	HIS	679	57.423	9.003	30.457	1.00	35.91
ATOM	5259	CB	HIS	679	58.348	8.294	31.439	1.00	35.05
ATOM	5260	CG	HIS	679	59.761	8.798	31.404	1.00	37.68
ATOM	5261	CD2	HIS	679	60.453	9.569	32.278	1.00	37.89
ATOM	5262	ND1	HIS	679	60.632	8.507	30.380	1.00	37.49
ATOM	5264	CE1	HIS	679	61.803	9.071	30.621	1.00	39.58
ATOM	5265	NE2	HIS	679	61.721	9.722	31.766	1.00	39.81
ATOM	5267	C	HIS	679	56.032	8.376	30.441	1.00	36.76
ATOM	5268	O	HIS	679	55.771	7.458	29.660	1.00	37.16
ATOM	5269	N	GLN	680	55.126	8.908	31.264	1.00	36.27
ATOM	5271	CA	GLN	680	53.754	8.407	31.332	1.00	37.71
ATOM	5272	CB	GLN	680	53.069	8.815	32.640	1.00	40.95
ATOM	5273	CG	GLN	680	53.645	8.128	33.884	1.00	45.23
ATOM	5274	CD	GLN	680	53.676	6.595	33.780	1.00	44.44
ATOM	5275	OE1	GLN	680	52.669	5.925	33.996	1.00	42.76
ATOM	5276	NE2	GLN	680	54.846	6.043	33.464	1.00	40.57
ATOM	5279	C	GLN	680	52.927	8.842	30.121	1.00	37.54

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ATOM	5280	O	GLN	680	51.950	8.185	29.765	1.00	37.93
ATOM	5281	N	SER	681	53.282	9.961	29.504	1.00	36.38
ATOM	5283	CA	SER	681	52.563	10.367	28.306	1.00	38.05
ATOM	5284	CB	SER	681	52.857	11.819	27.940	1.00	41.41
ATOM	5285	OG	SER	681	54.239	12.069	27.938	1.00	42.92
ATOM	5287	C	SER	681	52.991	9.421	27.178	1.00	37.92
ATOM	5288	O	SER	681	52.205	9.148	26.263	1.00	37.21
ATOM	5289	N	ASP	682	54.237	8.932	27.248	1.00	34.77
ATOM	5291	CA	ASP	682	54.750	7.972	26.267	1.00	31.99
ATOM	5292	CB	ASP	682	56.243	7.683	26.481	1.00	31.08
ATOM	5293	CG	ASP	682	57.165	8.638	25.721	1.00	33.63
ATOM	5294	OD1	ASP	682	58.386	8.503	25.920	1.00	32.35
ATOM	5295	OD2	ASP	682	56.707	9.500	24.930	1.00	29.46
ATOM	5296	C	ASP	682	53.969	6.672	26.457	1.00	31.54
ATOM	5297	O	ASP	682	53.675	5.971	25.493	1.00	29.94
ATOM	5298	N	VAL	683	53.677	6.334	27.712	1.00	30.48
ATOM	5300	CA	VAL	683	52.913	5.126	28.023	1.00	32.94
ATOM	5301	CB	VAL	683	52.731	4.939	29.572	1.00	33.94
ATOM	5302	CG1	VAL	683	51.635	3.905	29.872	1.00	32.71
ATOM	5303	CG2	VAL	683	54.042	4.474	30.209	1.00	27.41
ATOM	5304	C	VAL	683	51.545	5.164	27.299	1.00	32.27
ATOM	5305	O	VAL	683	51.106	4.158	26.733	1.00	30.54
ATOM	5306	N	TRP	684	50.902	6.332	27.282	1.00	32.57
ATOM	5308	CA	TRP	684	49.616	6.477	26.600	1.00	32.76
ATOM	5309	CB	TRP	684	49.060	7.895	26.765	1.00	33.67
ATOM	5310	CG	TRP	684	47.855	8.210	25.891	1.00	38.22
ATOM	5311	CD2	TRP	684	46.503	8.435	26.328	1.00	39.96
ATOM	5312	CE2	TRP	684	45.734	8.735	25.177	1.00	39.59
ATOM	5313	CE3	TRP	684	45.869	8.416	27.578	1.00	39.26
ATOM	5314	CD1	TRP	684	47.842	8.373	24.528	1.00	39.02
ATOM	5315	NE1	TRP	684	46.576	8.687	24.096	1.00	38.42
ATOM	5317	CZ2	TRP	684	44.362	9.011	25.240	1.00	36.62
ATOM	5318	CZ3	TRP	684	44.502	8.691	27.641	1.00	40.70
ATOM	5319	CH2	TRP	684	43.766	8.982	26.475	1.00	40.57
ATOM	5320	C	TRP	684	49.819	6.158	25.125	1.00	31.98
ATOM	5321	O	TRP	684	49.066	5.367	24.557	1.00	32.43
ATOM	5322	N	SER	685	50.859	6.748	24.529	1.00	29.63
ATOM	5324	CA	SER	685	51.195	6.531	23.119	1.00	28.62
ATOM	5325	CB	SER	685	52.457	7.296	22.751	1.00	24.72
ATOM	5326	OG	SER	685	52.323	8.664	23.072	1.00	30.04
ATOM	5328	C	SER	685	51.414	5.055	22.825	1.00	27.91
ATOM	5329	O	SER	685	51.022	4.555	21.767	1.00	28.60
ATOM	5330	N	PHE	686	52.063	4.372	23.763	1.00	27.96
ATOM	5332	CA	PHE	686	52.333	2.947	23.662	1.00	27.03
ATOM	5333	CB	PHE	686	53.163	2.499	24.868	1.00	25.79
ATOM	5334	CG	PHE	686	53.440	1.029	24.890	1.00	26.25
ATOM	5335	CD1	PHE	686	54.252	0.451	23.923	1.00	27.32
ATOM	5336	CD2	PHE	686	52.839	0.208	25.841	1.00	26.22
ATOM	5337	CE1	PHE	686	54.464	-0.930	23.900	1.00	25.87
ATOM	5338	CE2	PHE	686	53.046	-1.170	25.828	1.00	24.37
ATOM	5339	CZ	PHE	686	53.856	-1.740	24.854	1.00	26.42
ATOM	5340	C	PHE	686	51.003	2.160	23.596	1.00	28.82
ATOM	5341	O	PHE	686	50.912	1.129	22.914	1.00	26.74
ATOM	5342	N	GLY	687	49.991	2.636	24.324	1.00	29.52

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ATOM	5344	CA	GLY	687	48.688	1.982	24.302	1.00	31.57
ATOM	5345	C	GLY	687	48.095	2.036	22.896	1.00	30.73
ATOM	5346	O	GLY	687	47.490	1.069	22.414	1.00	29.83
ATOM	5347	N	VAL	688	48.269	3.179	22.238	1.00	29.06
ATOM	5349	CA	VAL	688	47.777	3.350	20.879	1.00	28.93
ATOM	5350	CB	VAL	688	47.800	4.831	20.424	1.00	27.24
ATOM	5351	CG1	VAL	688	47.211	4.963	19.020	1.00	28.29
ATOM	5352	CG2	VAL	688	46.990	5.691	21.404	1.00	26.96
ATOM	5353	C	VAL	688	48.612	2.475	19.951	1.00	28.49
ATOM	5354	O	VAL	688	48.080	1.866	19.024	1.00	28.84
ATOM	5355	N	LEU	689	49.905	2.350	20.252	1.00	27.99
ATOM	5357	CA	LEU	689	50.804	1.512	19.461	1.00	26.14
ATOM	5358	CB	LEU	689	52.268	1.688	19.911	1.00	27.31
ATOM	5359	CG	LEU	689	53.368	1.014	19.065	1.00	26.60
ATOM	5360	CD1	LEU	689	54.688	1.767	19.175	1.00	28.19
ATOM	5361	CD2	LEU	689	53.567	-0.401	19.475	1.00	25.55
ATOM	5362	C	LEU	689	50.362	0.053	19.605	1.00	26.48
ATOM	5363	O	LEU	689	50.377	-0.686	18.626	1.00	27.06
ATOM	5364	N	LEU	690	49.953	-0.344	20.816	1.00	28.55
ATOM	5366	CA	LEU	690	49.465	-1.708	21.085	1.00	29.16
ATOM	5367	CB	LEU	690	49.070	-1.888	22.560	1.00	31.40
ATOM	5368	CG	LEU	690	50.114	-2.085	23.667	1.00	31.49
ATOM	5369	CD1	LEU	690	49.427	-2.028	25.026	1.00	34.09
ATOM	5370	CD2	LEU	690	50.821	-3.410	23.491	1.00	30.84
ATOM	5371	C	LEU	690	48.240	-1.958	20.220	1.00	26.51
ATOM	5372	O	LEU	690	48.088	-3.023	19.631	1.00	25.15
ATOM	5373	N	TRP	691	47.376	-0.954	20.139	1.00	28.51
ATOM	5375	CA	TRP	691	46.169	-1.049	19.319	1.00	29.56
ATOM	5376	CB	TRP	691	45.332	0.227	19.465	1.00	28.91
ATOM	5377	CG	TRP	691	43.992	0.169	18.759	1.00	30.95
ATOM	5378	CD2	TRP	691	43.718	0.556	17.406	1.00	29.87
ATOM	5379	CE2	TRP	691	42.337	0.367	17.189	1.00	31.97
ATOM	5380	CE3	TRP	691	44.505	1.049	16.358	1.00	27.72
ATOM	5381	CD1	TRP	691	42.796	-0.231	19.292	1.00	30.68
ATOM	5382	NE1	TRP	691	41.797	-0.111	18.355	1.00	33.68
ATOM	5384	CZ2	TRP	691	41.729	0.652	15.967	1.00	29.42
ATOM	5385	CZ3	TRP	691	43.906	1.327	15.154	1.00	27.13
ATOM	5386	CH2	TRP	691	42.523	1.129	14.965	1.00	29.18
ATOM	5387	C	TRP	691	46.564	-1.289	17.856	1.00	28.78
ATOM	5388	O	TRP	691	45.996	-2.156	17.194	1.00	27.64
ATOM	5389	N	GLU	692	47.564	-0.543	17.380	1.00	29.83
ATOM	5391	CA	GLU	692	48.078	-0.669	16.018	1.00	28.08
ATOM	5392	CB	GLU	692	49.267	0.262	15.790	1.00	26.40
ATOM	5393	CG	GLU	692	48.945	1.735	15.680	1.00	26.45
ATOM	5394	CD	GLU	692	50.183	2.561	15.369	1.00	29.47
ATOM	5395	OE1	GLU	692	50.938	2.886	16.320	1.00	29.66
ATOM	5396	OE2	GLU	692	50.413	2.875	14.182	1.00	29.44
ATOM	5397	C	GLU	692	48.563	-2.082	15.761	1.00	30.07
ATOM	5398	O	GLU	692	48.385	-2.612	14.665	1.00	30.18
ATOM	5399	N	ILE	693	49.244	-2.663	16.746	1.00	29.87
ATOM	5401	CA	ILE	693	49.754	-4.024	16.608	1.00	29.51
ATOM	5402	CB	ILE	693	50.632	-4.443	17.828	1.00	28.18
ATOM	5403	CG2	ILE	693	51.037	-5.907	17.706	1.00	27.45
ATOM	5404	CG1	ILE	693	51.907	-3.594	17.890	1.00	26.99

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ATOM	5405	CD1	ILE	693	52.663	-3.747	19.194	1.00	25.37
ATOM	5406	C	ILE	693	48.603	-5.023	16.452	1.00	29.21
ATOM	5407	O	ILE	693	48.568	-5.807	15.512	1.00	27.89
ATOM	5408	N	PHE	694	47.623	-4.942	17.336	1.00	31.33
ATOM	5410	CA	PHE	694	46.523	-5.888	17.279	1.00	34.41
ATOM	5411	CB	PHE	694	45.958	-6.114	18.687	1.00	35.37
ATOM	5412	CG	PHE	694	46.978	-6.717	19.621	1.00	35.60
ATOM	5413	CD1	PHE	694	47.606	-5.942	20.586	1.00	37.23
ATOM	5414	CD2	PHE	694	47.424	-8.024	19.426	1.00	35.59
ATOM	5415	CE1	PHE	694	48.669	-6.460	21.333	1.00	36.39
ATOM	5416	CE2	PHE	694	48.484	-8.546	20.170	1.00	35.34
ATOM	5417	CZ	PHE	694	49.110	-7.762	21.118	1.00	35.71
ATOM	5418	C	PHE	694	45.481	-5.715	16.176	1.00	34.41
ATOM	5419	O	PHE	694	44.623	-6.579	15.982	1.00	34.48
ATOM	5420	N	THR	695	45.617	-4.637	15.404	1.00	33.03
ATOM	5422	CA	THR	695	44.742	-4.379	14.263	1.00	31.81
ATOM	5423	CB	THR	695	44.113	-2.957	14.278	1.00	29.75
ATOM	5424	OG1	THR	695	45.142	-1.961	14.218	1.00	30.72
ATOM	5426	CG2	THR	695	43.254	-2.759	15.524	1.00	29.40
ATOM	5427	C	THR	695	45.596	-4.533	13.011	1.00	31.44
ATOM	5428	O	THR	695	45.153	-4.241	11.906	1.00	33.00
ATOM	5429	N	LEU	696	46.832	-4.987	13.209	1.00	31.24
ATOM	5431	CA	LEU	696	47.799	-5.199	12.134	1.00	31.36
ATOM	5432	CB	LEU	696	47.421	-6.418	11.291	1.00	33.53
ATOM	5433	CG	LEU	696	47.270	-7.741	12.042	1.00	33.00
ATOM	5434	CD1	LEU	696	47.010	-8.838	11.052	1.00	35.50
ATOM	5435	CD2	LEU	696	48.515	-8.061	12.830	1.00	36.09
ATOM	5436	C	LEU	696	48.066	-3.976	11.249	1.00	30.84
ATOM	5437	O	LEU	696	48.135	-4.067	10.024	1.00	28.23
ATOM	5438	N	GLY	697	48.302	-2.839	11.890	1.00	31.54
ATOM	5440	CA	GLY	697	48.591	-1.632	11.141	1.00	33.87
ATOM	5441	C	GLY	697	47.375	-0.765	10.924	1.00	32.77
ATOM	5442	O	GLY	697	47.322	0.042	9.994	1.00	33.90
ATOM	5443	N	GLY	698	46.392	-0.921	11.797	1.00	33.29
ATOM	5445	CA	GLY	698	45.187	-0.122	11.681	1.00	32.66
ATOM	5446	C	GLY	698	45.408	1.368	11.877	1.00	30.57
ATOM	5447	O	GLY	698	46.336	1.803	12.553	1.00	27.36
ATOM	5448	N	SER	699	44.517	2.148	11.285	1.00	30.92
ATOM	5450	CA	SER	699	44.552	3.595	11.376	1.00	32.19
ATOM	5451	CB	SER	699	44.062	4.202	10.058	1.00	34.24
ATOM	5452	OG	SER	699	44.019	5.616	10.123	1.00	38.67
ATOM	5454	C	SER	699	43.644	4.014	12.538	1.00	31.81
ATOM	5455	O	SER	699	42.431	3.759	12.525	1.00	31.39
ATOM	5456	N	PRO	700	44.228	4.597	13.594	1.00	31.82
ATOM	5457	CD	PRO	700	45.645	4.842	13.919	1.00	28.82
ATOM	5458	CA	PRO	700	43.353	4.992	14.697	1.00	31.31
ATOM	5459	CB	PRO	700	44.345	5.341	15.809	1.00	31.31
ATOM	5460	CG	PRO	700	45.552	5.800	15.061	1.00	30.41
ATOM	5461	C	PRO	700	42.484	6.170	14.295	1.00	31.19
ATOM	5462	O	PRO	700	42.899	7.021	13.510	1.00	29.93
ATOM	5463	N	TYR	701	41.235	6.144	14.736	1.00	32.69
ATOM	5465	CA	TYR	701	40.291	7.223	14.445	1.00	32.54
ATOM	5466	CB	TYR	701	40.650	8.416	15.323	1.00	34.47
ATOM	5467	CG	TYR	701	40.512	8.141	16.794	1.00	39.16

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ATOM	5468	CD1	TYR	701	41.542	8.433	17.683	1.00	44.31
ATOM	5469	CE1	TYR	701	41.372	8.241	19.060	1.00	46.65
ATOM	5470	CD2	TYR	701	39.321	7.642	17.307	1.00	41.21
ATOM	5471	CE2	TYR	701	39.147	7.447	18.657	1.00	45.05
ATOM	5472	CZ	TYR	701	40.164	7.750	19.535	1.00	47.24
ATOM	5473	OH	TYR	701	39.949	7.590	20.886	1.00	52.18
ATOM	5475	C	TYR	701	40.215	7.655	12.972	1.00	30.56
ATOM	5476	O	TYR	701	40.379	8.836	12.647	1.00	29.73
ATOM	5477	N	PRO	702	39.928	6.712	12.058	1.00	30.38
ATOM	5478	CD	PRO	702	39.659	5.278	12.261	1.00	30.22
ATOM	5479	CA	PRO	702	39.847	7.071	10.642	1.00	28.87
ATOM	5480	CB	PRO	702	39.693	5.722	9.948	1.00	29.63
ATOM	5481	CG	PRO	702	39.007	4.889	10.959	1.00	30.99
ATOM	5482	C	PRO	702	38.722	8.048	10.283	1.00	30.88
ATOM	5483	O	PRO	702	37.557	7.843	10.636	1.00	33.98
ATOM	5484	N	GLY	703	39.100	9.116	9.584	1.00	29.03
ATOM	5486	CA	GLY	703	38.154	10.134	9.169	1.00	28.98
ATOM	5487	C	GLY	703	37.893	11.169	10.244	1.00	29.69
ATOM	5488	O	GLY	703	37.074	12.068	10.048	1.00	31.71
ATOM	5489	N	VAL	704	38.579	11.040	11.378	1.00	30.74
ATOM	5491	CA	VAL	704	38.416	11.951	12.509	1.00	32.06
ATOM	5492	CB	VAL	704	38.582	11.208	13.860	1.00	31.70
ATOM	5493	CG1	VAL	704	38.522	12.197	15.044	1.00	30.29
ATOM	5494	CG2	VAL	704	37.506	10.144	14.005	1.00	31.56
ATOM	5495	C	VAL	704	39.430	13.087	12.449	1.00	33.72
ATOM	5496	O	VAL	704	40.634	12.867	12.548	1.00	35.31
ATOM	5497	N	PRO	705	38.957	14.309	12.200	1.00	34.23
ATOM	5498	CD	PRO	705	37.594	14.692	11.787	1.00	33.20
ATOM	5499	CA	PRO	705	39.875	15.443	12.135	1.00	33.73
ATOM	5500	CB	PRO	705	39.053	16.495	11.394	1.00	34.93
ATOM	5501	CG	PRO	705	37.647	16.187	11.831	1.00	36.93
ATOM	5502	C	PRO	705	40.280	15.879	13.543	1.00	33.25
ATOM	5503	O	PRO	705	39.651	15.490	14.532	1.00	31.71
ATOM	5504	N	VAL	706	41.322	16.697	13.623	1.00	34.46
ATOM	5506	CA	VAL	706	41.852	17.176	14.900	1.00	36.99
ATOM	5507	CB	VAL	706	42.923	18.261	14.687	1.00	39.01
ATOM	5508	CG1	VAL	706	43.577	18.618	16.017	1.00	40.33
ATOM	5509	CG2	VAL	706	43.961	17.786	13.673	1.00	38.61
ATOM	5510	C	VAL	706	40.826	17.716	15.895	1.00	35.65
ATOM	5511	O	VAL	706	40.823	17.319	17.065	1.00	33.55
ATOM	5512	N	GLU	707	39.955	18.605	15.426	1.00	36.74
ATOM	5514	CA	GLU	707	38.941	19.220	16.278	1.00	37.20
ATOM	5515	CB	GLU	707	38.129	20.242	15.482	1.00	38.98
ATOM	5516	C	GLU	707	38.014	18.188	16.900	1.00	38.46
ATOM	5517	O	GLU	707	37.634	18.295	18.074	1.00	39.04
ATOM	5518	N	GLU	708	37.681	17.170	16.115	1.00	37.81
ATOM	5520	CA	GLU	708	36.802	16.105	16.571	1.00	37.70
ATOM	5521	CB	GLU	708	36.316	15.289	15.378	1.00	40.73
ATOM	5522	CG	GLU	708	35.459	16.091	14.413	1.00	43.44
ATOM	5523	CD	GLU	708	34.235	16.677	15.084	1.00	51.52
ATOM	5524	OE1	GLU	708	33.629	16.007	15.961	1.00	50.14
ATOM	5525	OE2	GLU	708	33.882	17.824	14.732	1.00	59.46
ATOM	5526	C	GLU	708	37.506	15.223	17.588	1.00	36.53
ATOM	5527	O	GLU	708	36.897	14.782	18.567	1.00	36.80

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ATOM	5528	N	LEU	709	38.799	14.993	17.376	1.00	35.69
ATOM	5530	CA	LEU	709	39.584	14.179	18.301	1.00	35.48
ATOM	5531	CB	LEU	709	41.039	14.044	17.830	1.00	34.84
ATOM	5532	CG	LEU	709	41.921	13.250	18.802	1.00	32.41
ATOM	5533	CD1	LEU	709	41.608	11.787	18.674	1.00	30.10
ATOM	5534	CD2	LEU	709	43.378	13.514	18.560	1.00	29.93
ATOM	5535	C	LEU	709	39.568	14.842	19.673	1.00	35.58
ATOM	5536	O	LEU	709	39.377	14.177	20.694	1.00	35.43
ATOM	5537	N	PHE	710	39.792	16.150	19.686	1.00	36.79
ATOM	5539	CA	PHE	710	39.800	16.918	20.927	1.00	40.58
ATOM	5540	CB	PHE	710	39.944	18.413	20.637	1.00	42.55
ATOM	5541	CG	PHE	710	41.308	18.808	20.162	1.00	46.38
ATOM	5542	CD1	PHE	710	42.392	17.942	20.313	1.00	47.29
ATOM	5543	CD2	PHE	710	41.515	20.050	19.580	1.00	47.93
ATOM	5544	CE1	PHE	710	43.659	18.312	19.892	1.00	51.21
ATOM	5545	CE2	PHE	710	42.781	20.435	19.155	1.00	50.89
ATOM	5546	CZ	PHE	710	43.859	19.562	19.312	1.00	53.31
ATOM	5547	C	PHE	710	38.517	16.676	21.694	1.00	40.14
ATOM	5548	O	PHE	710	38.543	16.446	22.898	1.00	39.86
ATOM	5549	N	LYS	711	37.399	16.705	20.977	1.00	41.02
ATOM	5551	CA	LYS	711	36.101	16.479	21.584	1.00	38.66
ATOM	5552	CB	LYS	711	34.985	16.803	20.580	1.00	40.75
ATOM	5553	CG	LYS	711	33.601	16.727	21.181	1.00	46.99
ATOM	5554	CD	LYS	711	32.522	17.174	20.218	1.00	50.71
ATOM	5555	CE	LYS	711	31.163	16.733	20.739	1.00	52.53
ATOM	5556	NZ	LYS	711	30.041	17.194	19.884	1.00	57.76
ATOM	5560	C	LYS	711	35.990	15.046	22.120	1.00	38.06
ATOM	5561	O	LYS	711	35.535	14.831	23.250	1.00	36.29
ATOM	5562	N	LEU	712	36.431	14.066	21.330	1.00	38.10
ATOM	5564	CA	LEU	712	36.392	12.662	21.764	1.00	38.69
ATOM	5565	CB	LEU	712	36.914	11.714	20.672	1.00	37.19
ATOM	5566	CG	LEU	712	36.070	11.436	19.424	1.00	34.73
ATOM	5567	CD1	LEU	712	36.814	10.453	18.524	1.00	35.54
ATOM	5568	CD2	LEU	712	34.709	10.872	19.818	1.00	30.90
ATOM	5569	C	LEU	712	37.230	12.472	23.021	1.00	39.62
ATOM	5570	O	LEU	712	36.843	11.745	23.940	1.00	39.44
ATOM	5571	N	LEU	713	38.398	13.101	23.044	1.00	40.10
ATOM	5573	CA	LEU	713	39.279	12.999	24.199	1.00	42.81
ATOM	5574	CB	LEU	713	40.606	13.716	23.924	1.00	41.70
ATOM	5575	CG	LEU	713	41.495	13.040	22.868	1.00	41.86
ATOM	5576	CD1	LEU	713	42.742	13.862	22.607	1.00	37.19
ATOM	5577	CD2	LEU	713	41.873	11.647	23.340	1.00	41.17
ATOM	5578	C	LEU	713	38.577	13.566	25.437	1.00	43.18
ATOM	5579	O	LEU	713	38.479	12.889	26.457	1.00	44.79
ATOM	5580	N	LYS	714	38.004	14.760	25.312	1.00	42.75
ATOM	5582	CA	LYS	714	37.301	15.389	26.425	1.00	43.70
ATOM	5583	CB	LYS	714	36.842	16.796	26.043	1.00	44.69
ATOM	5584	CG	LYS	714	38.001	17.746	25.836	1.00	47.92
ATOM	5585	CD	LYS	714	37.543	19.171	25.583	1.00	55.01
ATOM	5586	CE	LYS	714	38.733	20.077	25.238	1.00	59.44
ATOM	5587	NZ	LYS	714	39.773	20.132	26.320	1.00	60.10
ATOM	5591	C	LYS	714	36.127	14.557	26.940	1.00	43.94
ATOM	5592	O	LYS	714	35.843	14.551	28.140	1.00	44.20
ATOM	5593	N	GLU	715	35.477	13.819	26.046	1.00	43.29

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ATOM	5595	CA	GLU	715	34.350	12.979	26.435	1.00	42.29
ATOM	5596	CB	GLU	715	33.464	12.682	25.225	1.00	44.91
ATOM	5597	CG	GLU	715	32.913	13.916	24.522	1.00	51.62
ATOM	5598	CD	GLU	715	32.020	13.566	23.332	1.00	55.01
ATOM	5599	OE1	GLU	715	32.343	12.605	22.596	1.00	58.09
ATOM	5600	OE2	GLU	715	30.992	14.251	23.136	1.00	55.83
ATOM	5601	C	GLU	715	34.806	11.665	27.064	1.00	41.07
ATOM	5602	O	GLU	715	33.982	10.825	27.421	1.00	38.01
ATOM	5603	N	GLY	716	36.118	11.476	27.182	1.00	41.11
ATOM	5605	CA	GLY	716	36.642	10.252	27.770	1.00	39.69
ATOM	5606	C	GLY	716	36.510	9.054	26.847	1.00	39.64
ATOM	5607	O	GLY	716	36.562	7.904	27.290	1.00	36.71
ATOM	5608	N	HIS	717	36.359	9.335	25.554	1.00	41.95
ATOM	5610	CA	HIS	717	36.215	8.300	24.541	1.00	43.32
ATOM	5611	CB	HIS	717	35.859	8.918	23.183	1.00	43.38
ATOM	5612	CG	HIS	717	35.813	7.926	22.060	1.00	44.79
ATOM	5613	CD2	HIS	717	34.802	7.152	21.596	1.00	44.64
ATOM	5614	ND1	HIS	717	36.912	7.625	21.285	1.00	46.21
ATOM	5616	CE1	HIS	717	36.584	6.708	20.392	1.00	46.21
ATOM	5617	NE2	HIS	717	35.307	6.404	20.561	1.00	45.55
ATOM	5619	C	HIS	717	37.485	7.481	24.403	1.00	43.90
ATOM	5620	O	HIS	717	38.581	8.031	24.327	1.00	45.45
ATOM	5621	N	ARG	718	37.304	6.169	24.289	1.00	43.44
ATOM	5623	CA	ARG	718	38.387	5.207	24.139	1.00	42.68
ATOM	5624	CB	ARG	718	38.500	4.361	25.412	1.00	41.00
ATOM	5625	CG	ARG	718	38.844	5.165	26.658	1.00	40.09
ATOM	5626	CD	ARG	718	40.214	5.825	26.495	1.00	41.06
ATOM	5627	NE	ARG	718	40.658	6.549	27.685	1.00	39.51
ATOM	5629	CZ	ARG	718	40.521	7.861	27.862	1.00	39.90
ATOM	5630	NH1	ARG	718	39.940	8.608	26.931	1.00	36.48
ATOM	5633	NH2	ARG	718	41.024	8.443	28.946	1.00	42.06
ATOM	5636	C	ARG	718	38.080	4.308	22.927	1.00	43.91
ATOM	5637	O	ARG	718	36.911	4.007	22.650	1.00	44.40
ATOM	5638	N	MET	719	39.113	3.933	22.174	1.00	42.56
ATOM	5640	CA	MET	719	38.928	3.079	21.004	1.00	42.82
ATOM	5641	CB	MET	719	40.219	2.964	20.181	1.00	42.59
ATOM	5642	CG	MET	719	40.595	4.221	19.413	1.00	41.15
ATOM	5643	SD	MET	719	42.093	4.079	18.400	1.00	44.11
ATOM	5644	CE	MET	719	43.323	3.949	19.613	1.00	41.33
ATOM	5645	C	MET	719	38.460	1.694	21.432	1.00	44.74
ATOM	5646	O	MET	719	38.822	1.216	22.516	1.00	41.56
ATOM	5647	N	ASP	720	37.635	1.075	20.582	1.00	45.50
ATOM	5649	CA	ASP	720	37.090	-0.265	20.824	1.00	45.51
ATOM	5650	CB	ASP	720	36.077	-0.660	19.733	1.00	48.60
ATOM	5651	CG	ASP	720	34.811	0.181	19.749	1.00	53.03
ATOM	5652	OD1	ASP	720	34.678	1.082	20.612	1.00	59.61
ATOM	5653	OD2	ASP	720	33.943	-0.067	18.880	1.00	50.58
ATOM	5654	C	ASP	720	38.177	-1.329	20.823	1.00	43.64
ATOM	5655	O	ASP	720	39.235	-1.172	20.199	1.00	43.66
ATOM	5656	N	LYS	721	37.876	-2.436	21.487	1.00	42.90
ATOM	5658	CA	LYS	721	38.784	-3.565	21.555	1.00	42.96
ATOM	5659	CB	LYS	721	38.278	-4.565	22.587	1.00	42.51
ATOM	5660	CG	LYS	721	39.000	-5.888	22.570	1.00	47.68
ATOM	5661	CD	LYS	721	38.445	-6.805	23.628	1.00	51.61

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ATOM	5662	CE	LYS	721	38.450	-8.246	23.163	1.00	54.96
ATOM	5663	NZ	LYS	721	38.165	-9.190	24.282	1.00	59.67
ATOM	5667	C	LYS	721	38.825	-4.215	20.182	1.00	43.05
ATOM	5668	O	LYS	721	37.779	-4.577	19.625	1.00	46.08
ATOM	5669	N	PRO	722	40.025	-4.348	19.601	1.00	43.22
ATOM	5670	CD	PRO	722	41.337	-3.872	20.067	1.00	43.52
ATOM	5671	CA	PRO	722	40.139	-4.968	18.275	1.00	41.04
ATOM	5672	CB	PRO	722	41.631	-4.856	17.965	1.00	40.87
ATOM	5673	CG	PRO	722	42.074	-3.682	18.764	1.00	42.22
ATOM	5674	C	PRO	722	39.726	-6.427	18.346	1.00	39.64
ATOM	5675	O	PRO	722	39.730	-7.023	19.425	1.00	37.12
ATOM	5676	N	SER	723	39.311	-6.982	17.212	1.00	40.36
ATOM	5678	CA	SER	723	38.947	-8.389	17.158	1.00	41.41
ATOM	5679	CB	SER	723	38.205	-8.707	15.865	1.00	38.26
ATOM	5680	OG	SER	723	39.049	-8.520	14.749	1.00	43.87
ATOM	5682	C	SER	723	40.294	-9.102	17.191	1.00	41.54
ATOM	5683	O	SER	723	41.284	-8.575	16.703	1.00	40.90
ATOM	5684	N	ASN	724	40.338	-10.300	17.750	1.00	44.89
ATOM	5686	CA	ASN	724	41.598	-11.019	17.853	1.00	48.14
ATOM	5687	CB	ASN	724	42.256	-11.202	16.476	1.00	52.43
ATOM	5688	CG	ASN	724	41.682	-12.374	15.715	1.00	57.29
ATOM	5689	OD1	ASN	724	41.637	-13.492	16.225	1.00	61.96
ATOM	5690	ND2	ASN	724	41.218	-12.125	14.500	1.00	60.91
ATOM	5693	C	ASN	724	42.509	-10.255	18.811	1.00	48.17
ATOM	5694	O	ASN	724	43.648	-9.918	18.495	1.00	49.88
ATOM	5695	N	CYS	725	41.960	-9.935	19.973	1.00	47.12
ATOM	5697	CA	CYS	725	42.686	-9.238	21.010	1.00	46.17
ATOM	5698	CB	CYS	725	42.569	-7.717	20.862	1.00	44.83
ATOM	5699	SG	CYS	725	43.459	-6.813	22.159	1.00	42.51
ATOM	5700	C	CYS	725	42.017	-9.697	22.294	1.00	45.78
ATOM	5701	O	CYS	725	40.803	-9.642	22.423	1.00	44.83
ATOM	5702	N	THR	726	42.810	-10.224	23.212	1.00	45.63
ATOM	5704	CA	THR	726	42.289	-10.711	24.482	1.00	45.47
ATOM	5705	CB	THR	726	43.351	-11.545	25.217	1.00	45.93
ATOM	5706	OG1	THR	726	44.307	-10.651	25.786	1.00	45.04
ATOM	5708	CG2	THR	726	44.061	-12.495	24.233	1.00	42.99
ATOM	5709	C	THR	726	41.858	-9.545	25.359	1.00	45.73
ATOM	5710	O	THR	726	42.368	-8.445	25.216	1.00	46.91
ATOM	5711	N	ASN	727	40.914	-9.789	26.257	1.00	45.93
ATOM	5713	CA	ASN	727	40.448	-8.736	27.141	1.00	47.85
ATOM	5714	CB	ASN	727	39.300	-9.237	28.022	1.00	54.88
ATOM	5715	CG	ASN	727	39.629	-10.544	28.731	1.00	65.11
ATOM	5716	OD1	ASN	727	40.737	-10.734	29.229	1.00	70.58
ATOM	5717	ND2	ASN	727	38.681	-11.472	28.735	1.00	69.68
ATOM	5720	C	ASN	727	41.591	-8.212	27.999	1.00	44.18
ATOM	5721	O	ASN	727	41.594	-7.047	28.390	1.00	41.35
ATOM	5722	N	GLU	728	42.572	-9.073	28.260	1.00	42.82
ATOM	5724	CA	GLU	728	43.725	-8.713	29.071	1.00	42.37
ATOM	5725	CB	GLU	728	44.573	-9.952	29.379	1.00	43.09
ATOM	5726	CG	GLU	728	45.806	-9.654	30.245	1.00	48.30
ATOM	5727	CD	GLU	728	46.643	-10.889	30.568	1.00	50.11
ATOM	5728	OE1	GLU	728	46.867	-11.732	29.668	1.00	47.98
ATOM	5729	OE2	GLU	728	47.085	-11.010	31.733	1.00	51.69
ATOM	5730	C	GLU	728	44.551	-7.652	28.356	1.00	39.57

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ATOM	5731	O	GLU	728	44.852	-6.605	28.933	1.00	39.30
ATOM	5732	N	LEU	729	44.872	-7.907	27.089	1.00	37.38
ATOM	5734	CA	LEU	729	45.655	-6.977	26.274	1.00	36.74
ATOM	5735	CB	LEU	729	46.027	-7.623	24.935	1.00	35.39
ATOM	5736	CG	LEU	729	47.137	-8.679	25.001	1.00	35.41
ATOM	5737	CD1	LEU	729	47.107	-9.553	23.766	1.00	35.69
ATOM	5738	CD2	LEU	729	48.505	-8.017	25.174	1.00	37.72
ATOM	5739	C	LEU	729	44.885	-5.679	26.050	1.00	35.52
ATOM	5740	O	LEU	729	45.467	-4.597	25.941	1.00	33.96
ATOM	5741	N	TYR	730	43.565	-5.779	26.000	1.00	32.90
ATOM	5743	CA	TYR	730	42.760	-4.598	25.812	1.00	32.41
ATOM	5744	CB	TYR	730	41.335	-4.981	25.398	1.00	32.16
ATOM	5745	CG	TYR	730	40.445	-3.787	25.172	1.00	34.93
ATOM	5746	CD1	TYR	730	40.769	-2.827	24.203	1.00	32.49
ATOM	5747	CE1	TYR	730	39.962	-1.716	23.994	1.00	32.80
ATOM	5748	CD2	TYR	730	39.282	-3.605	25.931	1.00	33.45
ATOM	5749	CE2	TYR	730	38.465	-2.496	25.728	1.00	34.81
ATOM	5750	CZ	TYR	730	38.814	-1.557	24.756	1.00	34.06
ATOM	5751	OH	TYR	730	38.009	-0.465	24.551	1.00	36.66
ATOM	5753	C	TYR	730	42.767	-3.788	27.107	1.00	33.48
ATOM	5754	O	TYR	730	42.837	-2.558	27.083	1.00	34.94
ATOM	5755	N	MET	731	42.698	-4.466	28.248	1.00	35.29
ATOM	5757	CA	MET	731	42.724	-3.755	29.525	1.00	38.38
ATOM	5758	CB	MET	731	42.465	-4.709	30.690	1.00	42.01
ATOM	5759	CG	MET	731	41.048	-5.264	30.702	1.00	53.67
ATOM	5760	SD	MET	731	39.785	-3.965	30.830	1.00	62.97
ATOM	5761	CE	MET	731	39.828	-3.688	32.641	1.00	61.83
ATOM	5762	C	MET	731	44.073	-3.049	29.670	1.00	34.52
ATOM	5763	O	MET	731	44.160	-1.958	30.232	1.00	33.23
ATOM	5764	N	MET	732	45.118	-3.669	29.134	1.00	33.93
ATOM	5766	CA	MET	732	46.445	-3.065	29.168	1.00	36.26
ATOM	5767	CB	MET	732	47.506	-3.995	28.565	1.00	35.56
ATOM	5768	CG	MET	732	48.935	-3.418	28.643	1.00	35.26
ATOM	5769	SD	MET	732	50.186	-4.522	28.001	1.00	30.46
ATOM	5770	CE	MET	732	50.480	-5.562	29.415	1.00	26.88
ATOM	5771	C	MET	732	46.369	-1.750	28.389	1.00	34.75
ATOM	5772	O	MET	732	46.827	-0.722	28.873	1.00	35.49
ATOM	5773	N	MET	733	45.741	-1.774	27.213	1.00	34.63
ATOM	5775	CA	MET	733	45.571	-0.566	26.413	1.00	32.79
ATOM	5776	CB	MET	733	44.787	-0.853	25.130	1.00	33.16
ATOM	5777	CG	MET	733	45.544	-1.601	24.047	1.00	32.32
ATOM	5778	SD	MET	733	44.421	-1.990	22.670	1.00	35.66
ATOM	5779	CE	MET	733	45.155	-3.496	22.068	1.00	29.47
ATOM	5780	C	MET	733	44.789	0.452	27.229	1.00	33.94
ATOM	5781	O	MET	733	45.176	1.619	27.318	1.00	35.72
ATOM	5782	N	ARG	734	43.679	0.018	27.818	1.00	33.73
ATOM	5784	CA	ARG	734	42.854	0.913	28.621	1.00	33.41
ATOM	5785	CB	ARG	734	41.586	0.197	29.095	1.00	33.42
ATOM	5786	CG	ARG	734	40.726	-0.335	27.950	1.00	34.26
ATOM	5787	CD	ARG	734	40.256	0.783	27.043	1.00	37.70
ATOM	5788	NE	ARG	734	39.416	1.745	27.750	1.00	43.98
ATOM	5790	CZ	ARG	734	38.092	1.661	27.844	1.00	46.43
ATOM	5791	NH1	ARG	734	37.439	0.660	27.268	1.00	48.63
ATOM	5794	NH2	ARG	734	37.420	2.571	28.530	1.00	44.65

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ATOM	5797	C	ARG	734	43.660	1.458	29.793	1.00	32.12
ATOM	5798	O	ARG	734	43.492	2.610	30.180	1.00	35.37
ATOM	5799	N	ASP	735	44.566	0.646	30.327	1.00	33.75
ATOM	5801	CA	ASP	735	45.438	1.076	31.433	1.00	36.72
ATOM	5802	CB	ASP	735	46.379	-0.055	31.857	1.00	42.71
ATOM	5803	CG	ASP	735	45.722	-1.052	32.774	1.00	47.31
ATOM	5804	OD1	ASP	735	46.124	-2.241	32.720	1.00	50.99
ATOM	5805	OD2	ASP	735	44.824	-0.646	33.552	1.00	48.45
ATOM	5806	C	ASP	735	46.291	2.251	30.972	1.00	34.25
ATOM	5807	O	ASP	735	46.376	3.286	31.648	1.00	34.31
ATOM	5808	N	CYS	736	46.927	2.064	29.816	1.00	31.85
ATOM	5810	CA	CYS	736	47.780	3.077	29.204	1.00	29.93
ATOM	5811	CB	CYS	736	48.413	2.545	27.921	1.00	24.97
ATOM	5812	SG	CYS	736	49.504	1.159	28.180	1.00	31.35
ATOM	5813	C	CYS	736	46.994	4.325	28.885	1.00	31.62
ATOM	5814	O	CYS	736	47.562	5.416	28.823	1.00	30.73
ATOM	5815	N	TRP	737	45.680	4.174	28.711	1.00	35.03
ATOM	5817	CA	TRP	737	44.812	5.308	28.395	1.00	36.35
ATOM	5818	CB	TRP	737	43.808	4.927	27.297	1.00	36.43
ATOM	5819	CG	TRP	737	44.451	4.487	26.010	1.00	34.34
ATOM	5820	CD2	TRP	737	43.914	3.565	25.052	1.00	34.81
ATOM	5821	CE2	TRP	737	44.852	3.461	23.999	1.00	33.92
ATOM	5822	CE3	TRP	737	42.730	2.816	24.980	1.00	33.06
ATOM	5823	CD1	TRP	737	45.659	4.890	25.514	1.00	35.19
ATOM	5824	NE1	TRP	737	45.907	4.279	24.309	1.00	35.00
ATOM	5826	CZ2	TRP	737	44.644	2.633	22.886	1.00	33.45
ATOM	5827	CZ3	TRP	737	42.527	1.991	23.876	1.00	32.92
ATOM	5828	CH2	TRP	737	43.480	1.909	22.844	1.00	30.45
ATOM	5829	C	TRP	737	44.080	5.895	29.609	1.00	37.23
ATOM	5830	O	TRP	737	43.047	6.551	29.474	1.00	37.44
ATOM	5831	N	HIS	738	44.624	5.681	30.798	1.00	41.45
ATOM	5833	CA	HIS	738	44.006	6.208	32.008	1.00	41.52
ATOM	5834	CB	HIS	738	44.675	5.635	33.258	1.00	41.23
ATOM	5835	CG	HIS	738	43.925	5.924	34.522	1.00	43.31
ATOM	5836	CD2	HIS	738	43.618	7.096	35.126	1.00	41.58
ATOM	5837	ND1	HIS	738	43.338	4.935	35.279	1.00	44.22
ATOM	5839	CE1	HIS	738	42.693	5.487	36.294	1.00	46.62
ATOM	5840	NE2	HIS	738	42.848	6.798	36.223	1.00	43.99
ATOM	5842	C	HIS	738	44.118	7.726	32.015	1.00	41.75
ATOM	5843	O	HIS	738	45.179	8.268	31.731	1.00	40.84
ATOM	5844	N	ALA	739	43.025	8.405	32.352	1.00	42.47
ATOM	5846	CA	ALA	739	43.004	9.873	32.398	1.00	44.58
ATOM	5847	CB	ALA	739	41.629	10.361	32.825	1.00	48.19
ATOM	5848	C	ALA	739	44.081	10.467	33.317	1.00	45.12
ATOM	5849	O	ALA	739	44.653	11.510	33.020	1.00	45.66
ATOM	5850	N	VAL	740	44.262	9.852	34.481	1.00	46.64
ATOM	5852	CA	VAL	740	45.278	10.273	35.453	1.00	46.78
ATOM	5853	CB	VAL	740	44.867	9.893	36.888	1.00	47.74
ATOM	5854	CG1	VAL	740	45.919	10.372	37.890	1.00	49.35
ATOM	5855	CG2	VAL	740	43.515	10.495	37.211	1.00	47.89
ATOM	5856	C	VAL	740	46.601	9.573	35.121	1.00	45.24
ATOM	5857	O	VAL	740	46.754	8.362	35.347	1.00	45.01
ATOM	5858	N	PRO	741	47.588	10.335	34.637	1.00	43.46
ATOM	5859	CD	PRO	741	47.536	11.794	34.437	1.00	43.51

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ATOM	5860	CA	PRO	741	48.905	9.804	34.266	1.00	46.22
ATOM	5861	CB	PRO	741	49.701	11.070	33.942	1.00	45.32
ATOM	5862	CG	PRO	741	48.632	12.010	33.426	1.00	42.81
ATOM	5863	C	PRO	741	49.588	8.936	35.328	1.00	47.45
ATOM	5864	O	PRO	741	50.245	7.950	34.994	1.00	45.12
ATOM	5865	N	SER	742	49.394	9.280	36.601	1.00	48.78
ATOM	5867	CA	SER	742	49.994	8.532	37.703	1.00	48.76
ATOM	5868	CB	SER	742	49.845	9.317	39.012	1.00	51.11
ATOM	5869	OG	SER	742	48.482	9.488	39.373	1.00	53.50
ATOM	5871	C	SER	742	49.376	7.150	37.867	1.00	47.77
ATOM	5872	O	SER	742	49.932	6.283	38.539	1.00	47.31
ATOM	5873	N	GLN	743	48.199	6.962	37.284	1.00	47.57
ATOM	5875	CA	GLN	743	47.511	5.689	37.384	1.00	47.14
ATOM	5876	CB	GLN	743	46.004	5.918	37.531	1.00	50.16
ATOM	5877	CG	GLN	743	45.438	5.447	38.871	1.00	54.69
ATOM	5878	CD	GLN	743	46.239	5.964	40.051	1.00	57.62
ATOM	5879	OE1	GLN	743	46.898	5.196	40.749	1.00	59.09
ATOM	5880	NE2	GLN	743	46.202	7.277	40.268	1.00	59.45
ATOM	5883	C	GLN	743	47.816	4.774	36.212	1.00	44.41
ATOM	5884	O	GLN	743	47.365	3.627	36.182	1.00	44.39
ATOM	5885	N	ARG	744	48.515	5.305	35.212	1.00	42.87
ATOM	5887	CA	ARG	744	48.902	4.506	34.046	1.00	41.45
ATOM	5888	CB	ARG	744	49.350	5.397	32.883	1.00	37.34
ATOM	5889	CG	ARG	744	48.316	6.380	32.412	1.00	32.30
ATOM	5890	CD	ARG	744	48.854	7.207	31.270	1.00	31.37
ATOM	5891	NE	ARG	744	47.921	8.276	30.946	1.00	36.76
ATOM	5893	CZ	ARG	744	48.271	9.492	30.543	1.00	39.88
ATOM	5894	NH1	ARG	744	49.553	9.813	30.399	1.00	39.94
ATOM	5897	NH2	ARG	744	47.330	10.404	30.322	1.00	39.12
ATOM	5900	C	ARG	744	50.068	3.616	34.471	1.00	41.40
ATOM	5901	O	ARG	744	50.813	3.945	35.405	1.00	42.84
ATOM	5902	N	PRO	745	50.203	2.441	33.849	1.00	40.11
ATOM	5903	CD	PRO	745	49.345	1.739	32.876	1.00	39.91
ATOM	5904	CA	PRO	745	51.332	1.607	34.266	1.00	38.58
ATOM	5905	CB	PRO	745	51.019	0.261	33.605	1.00	37.46
ATOM	5906	CG	PRO	745	50.250	0.645	32.377	1.00	37.41
ATOM	5907	C	PRO	745	52.640	2.202	33.750	1.00	37.73
ATOM	5908	O	PRO	745	52.634	3.027	32.835	1.00	37.71
ATOM	5909	N	THR	746	53.753	1.843	34.373	1.00	35.90
ATOM	5911	CA	THR	746	55.050	2.328	33.913	1.00	34.77
ATOM	5912	CB	THR	746	56.085	2.380	35.075	1.00	33.85
ATOM	5913	OG1	THR	746	56.296	1.059	35.602	1.00	33.92
ATOM	5915	CG2	THR	746	55.605	3.302	36.177	1.00	32.17
ATOM	5916	C	THR	746	55.544	1.327	32.870	1.00	32.69
ATOM	5917	O	THR	746	55.026	0.213	32.795	1.00	31.56
ATOM	5918	N	PHE	747	56.538	1.708	32.066	1.00	34.04
ATOM	5920	CA	PHE	747	57.093	0.782	31.083	1.00	31.74
ATOM	5921	CB	PHE	747	58.121	1.472	30.193	1.00	30.55
ATOM	5922	CG	PHE	747	57.504	2.287	29.096	1.00	29.40
ATOM	5923	CD1	PHE	747	56.772	1.666	28.092	1.00	28.24
ATOM	5924	CD2	PHE	747	57.609	3.667	29.091	1.00	27.50
ATOM	5925	CE1	PHE	747	56.170	2.407	27.100	1.00	24.35
ATOM	5926	CE2	PHE	747	57.001	4.413	28.091	1.00	29.27
ATOM	5927	CZ	PHE	747	56.276	3.776	27.103	1.00	25.73

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ATOM	5928	C	PHE	747	57.714	-0.413	31.782	1.00	31.92
ATOM	5929	O	PHE	747	57.727	-1.514	31.243	1.00	32.46
ATOM	5930	N	LYS	748	58.233	-0.199	32.986	1.00	33.47
ATOM	5932	CA	LYS	748	58.816	-1.302	33.733	1.00	35.57
ATOM	5933	CB	LYS	748	59.468	-0.800	35.026	1.00	39.42
ATOM	5934	CG	LYS	748	60.083	-1.923	35.861	1.00	46.49
ATOM	5935	CD	LYS	748	60.817	-1.407	37.103	1.00	50.69
ATOM	5936	CE	LYS	748	61.253	-2.574	37.999	1.00	52.57
ATOM	5937	NZ	LYS	748	62.072	-2.129	39.155	1.00	56.45
ATOM	5941	C	LYS	748	57.700	-2.318	34.028	1.00	35.58
ATOM	5942	O	LYS	748	57.898	-3.526	33.871	1.00	34.72
ATOM	5943	N	GLN	749	56.522	-1.818	34.411	1.00	35.59
ATOM	5945	CA	GLN	749	55.369	-2.684	34.692	1.00	38.20
ATOM	5946	CB	GLN	749	54.154	-1.872	35.162	1.00	42.73
ATOM	5947	CG	GLN	749	54.264	-1.171	36.499	1.00	49.30
ATOM	5948	CD	GLN	749	53.060	-0.282	36.761	1.00	53.13
ATOM	5949	OE1	GLN	749	53.194	0.915	37.023	1.00	52.71
ATOM	5950	NE2	GLN	749	51.873	-0.856	36.644	1.00	58.54
ATOM	5953	C	GLN	749	54.954	-3.392	33.409	1.00	36.16
ATOM	5954	O	GLN	749	54.745	-4.605	33.393	1.00	36.67
ATOM	5955	N	LEU	750	54.801	-2.609	32.342	1.00	35.83
ATOM	5957	CA	LEU	750	54.381	-3.117	31.037	1.00	34.49
ATOM	5958	CB	LEU	750	54.324	-1.988	30.004	1.00	32.49
ATOM	5959	CG	LEU	750	53.206	-0.958	30.188	1.00	31.94
ATOM	5960	CD1	LEU	750	53.411	0.230	29.267	1.00	30.45
ATOM	5961	CD2	LEU	750	51.859	-1.610	29.933	1.00	29.30
ATOM	5962	C	LEU	750	55.294	-4.214	30.559	1.00	33.87
ATOM	5963	O	LEU	750	54.828	-5.208	30.027	1.00	34.72
ATOM	5964	N	VAL	751	56.598	-4.038	30.759	1.00	36.12
ATOM	5966	CA	VAL	751	57.585	-5.045	30.363	1.00	34.50
ATOM	5967	CB	VAL	751	59.054	-4.532	30.559	1.00	31.96
ATOM	5968	CG1	VAL	751	60.052	-5.646	30.308	1.00	30.24
ATOM	5969	CG2	VAL	751	59.342	-3.386	29.604	1.00	28.02
ATOM	5970	C	VAL	751	57.349	-6.321	31.182	1.00	36.11
ATOM	5971	O	VAL	751	57.333	-7.422	30.638	1.00	36.45
ATOM	5972	N	GLU	752	57.107	-6.165	32.479	1.00	37.83
ATOM	5974	CA	GLU	752	56.869	-7.326	33.331	1.00	41.47
ATOM	5975	CB	GLU	752	56.800	-6.910	34.804	1.00	43.03
ATOM	5976	CG	GLU	752	58.122	-6.305	35.263	1.00	52.52
ATOM	5977	CD	GLU	752	58.251	-6.176	36.761	1.00	57.18
ATOM	5978	OE1	GLU	752	58.600	-5.068	37.233	1.00	58.11
ATOM	5979	OE2	GLU	752	58.032	-7.191	37.461	1.00	61.59
ATOM	5980	C	GLU	752	55.623	-8.097	32.890	1.00	40.16
ATOM	5981	O	GLU	752	55.689	-9.308	32.642	1.00	39.75
ATOM	5982	N	ASP	753	54.524	-7.376	32.696	1.00	40.06
ATOM	5984	CA	ASP	753	53.275	-7.982	32.264	1.00	39.73
ATOM	5985	CB	ASP	753	52.157	-6.947	32.247	1.00	41.00
ATOM	5986	CG	ASP	753	51.668	-6.591	33.640	1.00	45.17
ATOM	5987	OD1	ASP	753	51.753	-7.468	34.543	1.00	49.78
ATOM	5988	OD2	ASP	753	51.210	-5.439	33.829	1.00	45.51
ATOM	5989	C	ASP	753	53.396	-8.595	30.890	1.00	39.64
ATOM	5990	O	ASP	753	52.955	-9.720	30.674	1.00	41.84
ATOM	5991	N	LEU	754	53.998	-7.861	29.960	1.00	37.75
ATOM	5993	CA	LEU	754	54.161	-8.358	28.603	1.00	38.16

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ATOM	5994	CB	LEU	754	54.664	-7.261	27.664	1.00	36.95
ATOM	5995	CG	LEU	754	53.552	-6.270	27.307	1.00	36.64
ATOM	5996	CD1	LEU	754	54.141	-5.062	26.590	1.00	34.02
ATOM	5997	CD2	LEU	754	52.459	-6.968	26.465	1.00	34.13
ATOM	5998	C	LEU	754	55.070	-9.561	28.571	1.00	38.46
ATOM	5999	O	LEU	754	54.905	-10.451	27.740	1.00	39.95
ATOM	6000	N	ASP	755	56.014	-9.602	29.502	1.00	39.19
ATOM	6002	CA	ASP	755	56.930	-10.728	29.594	1.00	40.87
ATOM	6003	CB	ASP	755	57.956	-10.462	30.696	1.00	45.11
ATOM	6004	CG	ASP	755	59.128	-11.415	30.652	1.00	48.64
ATOM	6005	OD1	ASP	755	59.759	-11.612	31.711	1.00	54.27
ATOM	6006	OD2	ASP	755	59.432	-11.954	29.565	1.00	51.46
ATOM	6007	C	ASP	755	56.082	-11.952	29.947	1.00	40.67
ATOM	6008	O	ASP	755	56.152	-12.996	29.289	1.00	38.49
ATOM	6009	N	ARG	756	55.232	-11.771	30.955	1.00	40.06
ATOM	6011	CA	ARG	756	54.340	-12.817	31.437	1.00	40.07
ATOM	6012	CB	ARG	756	53.573	-12.316	32.661	1.00	40.24
ATOM	6013	CG	ARG	756	52.435	-13.217	33.138	1.00	42.12
ATOM	6014	CD	ARG	756	51.791	-12.631	34.389	1.00	42.33
ATOM	6015	NE	ARG	756	51.353	-11.247	34.186	1.00	46.68
ATOM	6017	CZ	ARG	756	50.295	-10.891	33.460	1.00	48.17
ATOM	6018	NH1	ARG	756	49.549	-11.818	32.866	1.00	46.64
ATOM	6021	NH2	ARG	756	49.998	-9.605	33.305	1.00	48.92
ATOM	6024	C	ARG	756	53.362	-13.275	30.364	1.00	40.19
ATOM	6025	O	ARG	756	53.247	-14.469	30.110	1.00	42.24
ATOM	6026	N	ILE	757	52.688	-12.327	29.717	1.00	38.18
ATOM	6028	CA	ILE	757	51.706	-12.649	28.683	1.00	38.40
ATOM	6029	CB	ILE	757	50.952	-11.382	28.187	1.00	36.55
ATOM	6030	CG2	ILE	757	49.952	-11.758	27.105	1.00	34.67
ATOM	6031	CG1	ILE	757	50.216	-10.726	29.364	1.00	34.65
ATOM	6032	CD1	ILE	757	49.554	-9.423	29.048	1.00	36.49
ATOM	6033	C	ILE	757	52.301	-13.400	27.500	1.00	39.19
ATOM	6034	O	ILE	757	51.709	-14.360	27.025	1.00	39.66
ATOM	6035	N	VAL	758	53.492	-12.996	27.061	1.00	42.36
ATOM	6037	CA	VAL	758	54.161	-13.645	25.937	1.00	43.15
ATOM	6038	CB	VAL	758	55.582	-13.052	25.682	1.00	41.72
ATOM	6039	CG1	VAL	758	56.308	-13.855	24.621	1.00	41.57
ATOM	6040	CG2	VAL	758	55.491	-11.619	25.229	1.00	40.06
ATOM	6041	C	VAL	758	54.299	-15.133	26.231	1.00	47.11
ATOM	6042	O	VAL	758	54.045	-15.971	25.369	1.00	48.62
ATOM	6043	N	ALA	759	54.695	-15.446	27.464	1.00	49.64
ATOM	6045	CA	ALA	759	54.879	-16.820	27.908	1.00	51.35
ATOM	6046	CB	ALA	759	55.423	-16.830	29.317	1.00	50.11
ATOM	6047	C	ALA	759	53.568	-17.598	27.850	1.00	54.72
ATOM	6048	O	ALA	759	53.520	-18.717	27.348	1.00	58.64
ATOM	6049	N	LEU	760	52.496	-16.983	28.329	1.00	54.84
ATOM	6051	CA	LEU	760	51.194	-17.628	28.343	1.00	55.87
ATOM	6052	CB	LEU	760	50.330	-17.034	29.459	1.00	56.85
ATOM	6053	CG	LEU	760	50.875	-17.165	30.885	1.00	56.80
ATOM	6054	CD1	LEU	760	49.991	-16.392	31.849	1.00	56.78
ATOM	6055	CD2	LEU	760	50.959	-18.631	31.289	1.00	57.78
ATOM	6056	C	LEU	760	50.454	-17.546	27.013	1.00	57.36
ATOM	6057	O	LEU	760	49.262	-17.859	26.944	1.00	57.65
ATOM	6058	N	THR	761	51.151	-17.134	25.956	1.00	58.71

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ATOM	6060	CA	THR	761	50.541	-17.025	24.630	1.00	59.04
ATOM	6061	CB	THR	761	50.839	-15.657	23.971	1.00	56.72
ATOM	6062	OG1	THR	761	50.287	-14.610	24.775	1.00	56.53
ATOM	6064	CG2	THR	761	50.213	-15.584	22.590	1.00	53.81
ATOM	6065	C	THR	761	51.049	-18.138	23.721	1.00	60.44
ATOM	6066	O	THR	761	52.255	-18.295	23.530	1.00	61.40
ATOM	6067	SG	CYS	1603	18.474	-8.976	20.202	0.50	37.82 PRT2
ATOM	6068	CG	MET	534	69.311	12.109	23.281	0.50	36.25 PRT2
ATOM	6069	SD	MET	534	69.286	12.958	24.867	0.50	42.66 PRT2
ATOM	6070	CE	MET	534	70.539	12.083	25.804	0.50	43.27 PRT2
ATOM	6071	SG	CYS	603	56.046	-7.949	16.446	0.50	36.47 PRT2
ATOM	2676	OH2	TIP3	1	71.794	25.061	2.660	1.00	24.53
ATOM	2679	OH2	TIP3	2	39.750	3.992	15.898	1.00	39.62
ATOM	2682	OH2	TIP3	3	83.809	19.717	10.596	1.00	28.26
ATOM	2685	OH2	TIP3	4	83.630	20.056	7.685	1.00	26.19
ATOM	2688	OH2	TIP3	5	75.073	16.616	6.785	1.00	26.48
ATOM	2691	OH2	TIP3	6	86.549	19.594	9.502	1.00	33.65
ATOM	2694	OH2	TIP3	7	51.913	11.060	24.263	1.00	35.55
ATOM	2697	OH2	TIP3	8	55.093	9.421	22.524	1.00	26.63
ATOM	2700	OH2	TIP3	9	57.161	4.614	32.443	1.00	29.69
ATOM	2703	OH2	TIP3	10	52.169	4.735	13.281	1.00	22.61
ATOM	2706	OH2	TIP3	11	41.110	5.543	22.764	1.00	41.60
ATOM	2709	OH2	TIP3	12	45.145	8.857	21.555	1.00	36.99
ATOM	2712	OH2	TIP3	13	64.465	-2.607	28.883	1.00	30.17
ATOM	2715	OH2	TIP3	14	76.944	13.287	23.954	1.00	32.94
ATOM	2718	OH2	TIP3	15	79.062	17.048	18.200	1.00	51.65
ATOM	2721	OH2	TIP3	16	83.066	11.657	15.958	1.00	25.12
ATOM	2724	OH2	TIP3	17	13.957	-9.951	0.095	1.00	26.02
ATOM	2727	OH2	TIP3	18	38.359	-0.001	5.000	1.00	37.43
ATOM	2730	OH2	TIP3	19	5.442	2.705	19.077	1.00	29.46
ATOM	2733	OH2	TIP3	20	27.008	6.166	4.885	1.00	25.05
ATOM	2736	OH2	TIP3	21	34.242	-1.725	16.911	1.00	52.12
ATOM	2739	OH2	TIP3	22	20.167	2.428	27.681	1.00	42.69
ATOM	2742	OH2	TIP3	23	50.794	-11.834	38.045	1.00	60.16
ATOM	2745	OH2	TIP3	24	17.261	-5.993	-1.757	1.00	25.88
ATOM	2748	OH2	TIP3	25	27.516	7.803	15.070	1.00	39.33
ATOM	2751	OH2	TIP3	26	31.574	0.146	6.684	1.00	35.78
ATOM	2754	OH2	TIP3	27	27.119	-12.972	27.844	1.00	43.66
ATOM	2757	OH2	TIP3	28	28.439	-17.074	13.203	1.00	36.44
ATOM	2760	OH2	TIP3	29	88.706	14.393	7.969	1.00	32.49
ATOM	2763	OH2	TIP3	30	-2.338	-3.424	11.295	1.00	49.20
ATOM	2766	OH2	TIP3	31	35.086	-4.130	18.836	1.00	37.83
ATOM	2769	OH2	TIP3	32	80.455	17.922	9.507	1.00	23.69
ATOM	2772	OH2	TIP3	33	5.538	3.619	10.835	1.00	29.13
ATOM	2775	OH2	TIP3	34	-10.685	5.290	11.288	1.00	24.40
ATOM	2778	OH2	TIP3	35	29.210	-8.799	20.241	1.00	46.52
ATOM	2781	OH2	TIP3	36	6.195	3.150	13.803	1.00	31.39
ATOM	2784	OH2	TIP3	37	31.898	2.830	0.154	1.00	40.17
ATOM	2787	OH2	TIP3	38	19.915	2.023	-3.939	1.00	31.34
ATOM	2790	OH2	TIP3	39	62.242	2.604	32.859	1.00	39.67
ATOM	2793	OH2	TIP3	40	21.231	-7.063	-3.900	1.00	23.55
ATOM	2796	OH2	TIP3	41	-15.809	8.838	22.610	1.00	36.02
ATOM	2799	OH2	TIP3	42	40.120	2.154	8.433	1.00	60.62
ATOM	2802	OH2	TIP3	43	19.583	11.128	-0.045	1.00	37.85

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ATOM	2805	OH2	TIP3	44	67.056	9.030	17.389	1.00	29.79
ATOM	2808	OH2	TIP3	45	87.772	18.919	18.595	1.00	48.44
ATOM	2811	OH2	TIP3	46	74.584	17.123	4.200	1.00	39.18
ATOM	2814	OH2	TIP3	47	29.365	16.707	10.560	1.00	34.11
ATOM	2817	OH2	TIP3	48	66.486	6.826	15.051	1.00	32.28
ATOM	2820	OH2	TIP3	49	85.008	21.441	5.731	1.00	23.97
ATOM	2823	OH2	TIP3	50	-4.572	2.912	3.173	1.00	28.05
ATOM	2826	OH2	TIP3	51	19.496	5.141	4.881	1.00	28.88
ATOM	2829	OH2	TIP3	52	67.492	3.490	10.902	1.00	33.57
ATOM	2832	OH2	TIP3	53	34.791	5.413	24.797	1.00	40.16
ATOM	2835	OH2	TIP3	54	34.787	-16.910	13.756	1.00	39.46
ATOM	2838	OH2	TIP3	55	59.972	7.450	27.870	1.00	31.56
ATOM	2841	OH2	TIP3	56	-7.139	-1.696	6.345	1.00	42.00
ATOM	2844	OH2	TIP3	57	54.998	11.953	25.360	1.00	42.05
ATOM	2847	OH2	TIP3	58	68.697	6.686	16.740	1.00	46.12
ATOM	2850	OH2	TIP3	59	73.750	20.885	19.041	1.00	32.26
ATOM	2853	OH2	TIP3	60	3.431	-8.270	-8.218	1.00	31.22
ATOM	2856	OH2	TIP3	61	37.904	10.790	5.612	1.00	33.72
ATOM	2859	OH2	TIP3	62	29.982	-9.545	-1.303	1.00	39.11
ATOM	2862	OH2	TIP3	63	66.918	1.757	8.678	1.00	34.68
ATOM	2865	OH2	TIP3	64	49.117	1.310	12.227	1.00	34.31
ATOM	2868	OH2	TIP3	65	41.246	3.987	29.033	1.00	34.55
ATOM	2871	OH2	TIP3	66	10.755	-12.957	1.167	1.00	42.14
ATOM	2874	OH2	TIP3	67	-1.184	-4.327	21.439	1.00	37.90
ATOM	2877	OH2	TIP3	68	30.349	16.267	13.265	1.00	55.23
ATOM	2880	OH2	TIP3	69	8.111	4.362	3.445	1.00	23.88
ATOM	2883	OH2	TIP3	70	73.131	18.780	22.628	1.00	40.20
ATOM	2886	OH2	TIP3	71	-7.949	-3.409	24.953	1.00	35.49
ATOM	2889	OH2	TIP3	72	66.379	-4.621	28.423	1.00	45.46
ATOM	2892	OH2	TIP3	73	21.506	-20.711	4.815	1.00	52.46
ATOM	2895	OH2	TIP3	74	59.539	-6.865	4.928	1.00	48.87
ATOM	2898	OH2	TIP3	75	16.565	-13.297	-3.008	1.00	51.80
ATOM	2901	OH2	TIP3	76	-15.235	7.385	4.428	1.00	29.13
ATOM	2904	OH2	TIP3	77	32.926	2.785	13.213	1.00	37.62
ATOM	2907	OH2	TIP3	78	0.246	-2.768	10.996	1.00	28.25
ATOM	2910	OH2	TIP3	79	17.495	2.354	5.447	1.00	23.63
ATOM	2913	OH2	TIP3	80	6.336	2.434	21.950	1.00	29.56
ATOM	2916	OH2	TIP3	81	27.374	3.628	6.163	1.00	34.06
ATOM	2919	OH2	TIP3	82	-8.708	6.263	9.522	1.00	30.34
ATOM	2922	OH2	TIP3	83	1.500	-1.935	8.721	1.00	27.61
ATOM	2925	OH2	TIP3	84	-4.825	-3.133	6.984	1.00	33.50
ATOM	2928	OH2	TIP3	85	17.513	2.839	1.966	1.00	24.27
ATOM	2931	OH2	TIP3	86	20.298	3.414	2.920	1.00	26.15
ATOM	2934	OH2	TIP3	87	0.488	-2.158	22.213	1.00	25.95
ATOM	2937	OH2	TIP3	88	19.939	-6.185	-1.553	1.00	19.14
ATOM	2940	OH2	TIP3	89	10.670	-15.654	6.839	1.00	33.36
ATOM	2943	OH2	TIP3	90	4.107	-12.003	11.805	1.00	33.92
ATOM	2946	OH2	TIP3	91	6.238	0.927	-3.342	1.00	23.31
ATOM	2949	OH2	TIP3	92	-13.563	1.438	5.472	1.00	27.86
ATOM	2952	OH2	TIP3	93	15.707	-7.454	0.106	1.00	26.69
ATOM	2955	OH2	TIP3	94	-1.856	-5.393	3.795	1.00	39.91
ATOM	2958	OH2	TIP3	95	12.654	4.928	-4.474	1.00	31.32
ATOM	2961	OH2	TIP3	96	69.774	27.363	2.127	1.00	35.86
ATOM	2964	OH2	TIP3	97	24.636	-13.192	0.040	1.00	48.53

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ATOM	2967	OH2	TIP3 98	60.453	-4.625	33.829	1.00	31.97
ATOM	2970	OH2	TIP3 99	10.513	5.719	3.487	1.00	38.90
ATOM	2973	OH2	TIP3 100	-9.499	-4.011	4.342	1.00	30.61
ATOM	2976	OH2	TIP3 101	73.056	-1.608	10.514	1.00	36.08
ATOM	2979	OH2	TIP3 102	-3.152	5.709	30.608	1.00	29.38
ATOM	2982	OH2	TIP3 103	36.630	0.702	11.792	1.00	47.80
ATOM	2985	OH2	TIP3 104	21.475	6.325	16.924	1.00	24.03
ATOM	2988	OH2	TIP3 105	31.272	0.656	19.432	1.00	53.74
ATOM	2991	OH2	TIP3 106	5.620	-8.417	22.266	1.00	51.90
ATOM	2994	OH2	TIP3 107	-13.144	8.294	17.464	1.00	35.23
ATOM	2997	OH2	TIP3 108	26.680	-10.556	-1.042	1.00	27.83
ATOM	3000	OH2	TIP3 109	24.149	1.846	18.172	1.00	30.90
ATOM	3003	OH2	TIP3 110	-1.943	12.643	3.558	1.00	33.82
ATOM	3006	OH2	TIP3 111	59.560	13.617	33.196	1.00	54.79
ATOM	3009	OH2	TIP3 112	4.351	-10.740	1.991	1.00	37.96
ATOM	3012	OH2	TIP3 113	8.396	2.913	0.958	1.00	29.64
ATOM	3015	OH2	TIP3 114	75.905	1.753	25.812	1.00	38.73
ATOM	3018	OH2	TIP3 115	48.783	15.535	14.189	1.00	35.24
ATOM	3021	OH2	TIP3 116	2.419	-11.312	9.146	1.00	32.85
ATOM	3024	OH2	TIP3 117	83.014	26.360	12.964	1.00	41.83
ATOM	3027	OH2	TIP3 118	8.761	-6.579	-3.252	1.00	42.78
ATOM	3030	OH2	TIP3 119	-8.417	4.493	4.305	1.00	28.32
ATOM	3033	OH2	TIP3 120	7.908	-13.690	8.639	1.00	33.73
ATOM	3036	OH2	TIP3 121	51.437	6.329	10.373	1.00	31.72
ATOM	3039	OH2	TIP3 122	20.660	3.686	15.591	1.00	32.37
ATOM	3042	OH2	TIP3 123	73.039	3.790	20.450	1.00	35.80
ATOM	3045	OH2	TIP3 124	5.155	-11.467	22.590	1.00	45.12
ATOM	3048	OH2	TIP3 125	34.172	2.412	16.576	1.00	41.90
ATOM	3051	OH2	TIP3 126	9.597	-11.905	7.083	1.00	24.83
ATOM	3054	OH2	TIP3 127	8.276	3.860	-1.622	1.00	35.46
ATOM	3057	OH2	TIP3 128	66.282	5.755	12.352	1.00	35.43
ATOM	3060	OH2	TIP3 129	7.377	6.932	2.982	1.00	40.68
ATOM	3063	OH2	TIP3 130	35.832	-1.778	0.201	1.00	34.99
ATOM	3066	OH2	TIP3 131	44.781	10.362	11.064	1.00	42.31
ATOM	3069	OH2	TIP3 132	27.790	-12.638	18.958	1.00	58.71
ATOM	3072	OH2	TIP3 133	45.221	11.540	21.428	1.00	36.75
ATOM	3075	OH2	TIP3 134	57.560	-10.846	14.099	1.00	52.90
ATOM	3078	OH2	TIP3 135	-3.354	15.001	16.515	1.00	37.81
ATOM	3081	OH2	TIP3 136	85.717	11.251	9.062	1.00	35.18
ATOM	3084	OH2	TIP3 137	12.951	-2.469	2.075	1.00	22.07
ATOM	3087	OH2	TIP3 138	75.645	3.486	20.527	1.00	38.01
ATOM	3090	OH2	TIP3 139	13.237	7.412	-2.649	1.00	33.50
ATOM	3093	OH2	TIP3 140	11.262	-9.970	0.974	1.00	26.14
ATOM	3096	OH2	TIP3 141	59.480	10.772	14.098	1.00	52.08
ATOM	3099	OH2	TIP3 142	13.869	-16.121	3.919	1.00	40.06
ATOM	3102	OH2	TIP3 143	-6.407	-3.413	16.641	1.00	44.38
ATOM	3105	OH2	TIP3 144	25.667	-12.645	3.411	1.00	48.28
ATOM	3108	OH2	TIP3 145	-16.282	10.641	6.423	1.00	40.94
ATOM	3111	OH2	TIP3 146	86.637	12.861	7.008	1.00	39.45
ATOM	3114	OH2	TIP3 147	32.082	-4.569	1.892	1.00	27.35
ATOM	3117	OH2	TIP3 148	44.809	7.627	11.670	1.00	35.65
ATOM	3120	OH2	TIP3 149	80.693	12.459	16.523	1.00	37.21
ATOM	3123	OH2	TIP3 150	2.941	-7.118	-1.805	1.00	38.43
ATOM	3126	OH2	TIP3 151	31.794	-6.086	20.704	1.00	42.80

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ATOM	3129	OH2	TIP3	152	74.770	-2.683	12.398	1.00	40.40
ATOM	3132	OH2	TIP3	153	7.731	6.640	-1.037	1.00	35.61
ATOM	3135	OH2	TIP3	154	71.617	5.599	21.838	1.00	40.14
ATOM	3138	OH2	TIP3	155	68.113	-4.968	8.886	1.00	34.38
ATOM	3141	OH2	TIP3	156	0.042	-9.364	7.055	1.00	33.08
ATOM	3144	OH2	TIP3	157	68.020	18.352	10.995	1.00	34.76
ATOM	3147	OH2	TIP3	158	3.795	8.550	4.533	1.00	34.69
ATOM	3150	OH2	TIP3	159	52.106	11.746	18.410	1.00	40.06
ATOM	3153	OH2	TIP3	160	6.414	3.927	16.889	1.00	37.07
ATOM	3156	OH2	TIP3	161	-10.282	6.603	4.715	1.00	38.48
ATOM	3159	OH2	TIP3	162	76.410	1.681	-0.781	1.00	42.87
ATOM	3162	OH2	TIP3	163	9.910	-12.046	17.157	1.00	32.79
ATOM	3165	OH2	TIP3	164	33.983	14.219	18.191	1.00	37.35
ATOM	3168	OH2	TIP3	165	2.330	-7.952	16.978	1.00	44.25
ATOM	3171	OH2	TIP3	166	29.701	1.780	5.987	1.00	39.86
ATOM	3174	OH2	TIP3	167	32.494	-17.319	11.798	1.00	38.46
ATOM	3177	OH2	TIP3	168	42.107	17.932	10.978	1.00	44.83
ATOM	3180	OH2	TIP3	169	87.822	10.537	5.568	1.00	54.30
ATOM	3183	OH2	TIP3	170	70.261	-4.143	25.064	1.00	44.75
ATOM	3186	OH2	TIP3	171	77.519	5.882	23.891	1.00	42.67
ATOM	3189	OH2	TIP3	172	-0.921	-8.166	4.521	1.00	45.91
ATOM	3192	OH2	TIP3	173	34.213	15.329	1.478	1.00	40.10
ATOM	3195	OH2	TIP3	174	-9.647	7.731	7.383	1.00	35.63
ATOM	3198	OH2	TIP3	175	11.619	5.799	7.440	1.00	36.36
ATOM	3201	OH2	TIP3	176	-8.709	13.964	13.507	1.00	51.97
ATOM	3204	OH2	TIP3	177	31.770	3.376	18.354	1.00	46.26
ATOM	3207	OH2	TIP3	178	-8.494	9.789	24.269	1.00	50.98
ATOM	3210	OH2	TIP3	179	-1.234	-6.253	15.622	1.00	38.47
ATOM	3213	OH2	TIP3	180	80.252	0.887	15.691	1.00	39.48
ATOM	3216	OH2	TIP3	181	67.248	20.272	-1.555	1.00	48.22
ATOM	3219	OH2	TIP3	182	-0.566	4.367	1.362	1.00	39.84
ATOM	3222	OH2	TIP3	183	0.120	6.523	2.615	1.00	33.11
ATOM	3225	OH2	TIP3	184	-1.496	8.789	1.237	1.00	41.03
ATOM	3228	OH2	TIP3	185	-5.143	9.130	2.236	1.00	40.47
ATOM	3231	OH2	TIP3	186	-7.275	10.106	3.833	1.00	40.55
ATOM	3234	OH2	TIP3	187	2.717	7.275	0.769	1.00	44.67
ATOM	3237	OH2	TIP3	188	5.176	10.645	8.459	1.00	34.48
ATOM	3240	OH2	TIP3	189	63.822	12.690	22.883	1.00	41.88
ATOM	3243	OH2	TIP3	190	79.109	1.028	18.201	1.00	46.40
ATOM	3246	OH2	TIP3	191	59.332	-11.681	7.236	1.00	63.45
ATOM	3249	OH2	TIP3	192	13.967	-1.218	-4.268	1.00	34.79
ATOM	3252	OH2	TIP3	193	59.444	2.867	33.368	1.00	41.00
ATOM	3255	OH2	TIP3	194	32.024	13.487	19.852	1.00	53.61
ATOM	3258	OH2	TIP3	195	72.101	16.218	22.802	1.00	44.03
ATOM	3261	OH2	TIP3	196	0.987	-8.546	14.474	1.00	41.38
ATOM	3264	OH2	TIP3	197	-0.491	5.461	30.372	1.00	38.51
ATOM	3267	OH2	TIP3	198	61.179	6.795	11.905	1.00	41.77
ATOM	3270	OH2	TIP3	199	-1.365	-4.128	27.656	1.00	50.98
ATOM	3273	OH2	TIP3	200	81.440	15.558	17.262	1.00	44.47
ATOM	3276	OH2	TIP3	201	-17.491	4.116	23.873	1.00	50.58
ATOM	3279	OH2	TIP3	202	27.546	10.513	14.499	1.00	39.06
ATOM	3282	OH2	TIP3	203	34.992	4.513	27.719	1.00	49.89
ATOM	3285	OH2	TIP3	204	-3.486	-4.591	9.171	1.00	49.53
ATOM	3288	OH2	TIP3	205	42.799	7.848	22.320	1.00	43.50

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ATOM	3291	OH2	TIP3	206	52.728	11.884	21.811	1.00	39.98
ATOM	3294	OH2	TIP3	207	26.706	14.069	19.833	1.00	46.68
ATOM	3297	OH2	TIP3	208	-7.154	8.907	6.444	1.00	42.83
ATOM	3300	OH2	TIP3	209	86.648	5.606	16.034	1.00	51.15
ATOM	3303	OH2	TIP3	210	54.879	15.840	20.379	1.00	50.23
ATOM	3306	OH2	TIP3	211	51.417	19.473	22.691	1.00	48.35
ATOM	3309	OH2	TIP3	212	20.102	6.924	7.085	1.00	38.15
ATOM	3312	OH2	TIP3	213	28.991	1.941	-3.570	1.00	47.39
ATOM	3315	OH2	TIP3	214	26.505	2.386	-4.633	1.00	46.48
ATOM	3318	OH2	TIP3	215	36.482	2.810	18.521	1.00	46.26
ATOM	3321	OH2	TIP3	216	16.941	-20.504	14.128	1.00	49.74
ATOM	3324	OH2	TIP3	217	28.572	-14.448	6.157	1.00	49.13
ATOM	3327	OH2	TIP3	218	31.380	1.471	-1.998	1.00	43.02
ATOM	3330	OH2	TIP3	219	10.065	-16.338	15.455	1.00	42.75
ATOM	3333	OH2	TIP3	220	7.350	-11.974	5.652	1.00	55.35
ATOM	3336	OH2	TIP3	221	-12.328	14.547	10.986	1.00	51.29
ATOM	3339	OH2	TIP3	222	11.186	9.609	-1.388	1.00	37.68
ATOM	3342	OH2	TIP3	223	11.389	12.276	-1.400	1.00	46.93
ATOM	3345	OH2	TIP3	224	34.202	13.069	-1.161	1.00	41.79
ATOM	3348	OH2	TIP3	225	31.303	17.822	7.853	1.00	48.21
ATOM	3351	OH2	TIP3	226	36.875	11.804	-2.106	1.00	59.03
ATOM	3354	OH2	TIP3	227	35.134	3.048	11.020	1.00	50.41
ATOM	3357	OH2	TIP3	228	63.950	13.409	26.627	1.00	43.40
ATOM	3360	OH2	TIP3	229	36.367	6.116	15.221	1.00	57.79
ATOM	3363	OH2	TIP3	230	90.606	4.355	6.342	1.00	47.53
ATOM	3366	OH2	TIP3	231	50.038	-11.673	10.767	1.00	56.90
ATOM	3369	OH2	TIP3	232	60.196	-10.144	16.590	1.00	51.61
ATOM	3372	OH2	TIP3	233	18.021	-21.179	7.008	1.00	49.93
ATOM	3375	OH2	TIP3	234	66.236	-1.218	30.583	1.00	39.55
ATOM	3378	OH2	TIP3	235	74.959	18.928	20.659	1.00	38.04
ATOM	3381	OH2	TIP3	236	-2.816	10.082	3.187	1.00	49.31
ATOM	3384	OH2	TIP3	237	5.894	-3.410	25.289	1.00	35.55
ATOM	3387	OH2	TIP3	238	35.784	6.047	12.543	1.00	41.96
ATOM	3390	OH2	TIP3	239	-5.400	16.537	14.180	1.00	43.13
ATOM	3393	OH2	TIP3	240	46.589	-11.622	26.970	1.00	43.71
ATOM	3396	OH2	TIP3	241	6.199	6.592	13.797	1.00	46.51
ATOM	3399	OH2	TIP3	242	-3.777	-5.158	20.907	1.00	42.08
ATOM	3402	OH2	TIP3	243	1.969	-3.711	-0.282	1.00	37.38
ATOM	3405	OH2	TIP3	244	86.200	11.629	22.877	1.00	56.51
ATOM	3408	OH2	TIP3	245	10.557	7.565	5.514	1.00	47.58
ATOM	3411	OH2	TIP3	246	4.802	8.149	2.136	1.00	50.70
ATOM	3414	OH2	TIP3	247	64.590	-8.128	20.596	1.00	43.65
ATOM	3417	OH2	TIP3	248	11.346	-17.840	13.283	1.00	47.64
ATOM	3420	OH2	TIP3	249	42.116	-6.808	14.953	1.00	53.79
ATOM	3423	OH2	TIP3	250	2.745	-4.054	22.128	1.00	60.88
ATOM	3426	OH2	TIP3	251	71.999	1.177	-2.124	1.00	47.90
ATOM	3429	OH2	TIP3	252	50.328	-3.210	33.068	1.00	57.01
ATOM	3435	OH2	TIP3	253	57.838	9.337	11.631	1.00	52.55
ATOM	3438	OH2	TIP3	254	43.373	20.489	30.490	1.00	51.97
ATOM	3441	OH2	TIP3	255	67.045	16.529	15.793	1.00	49.02
ATOM	3444	OH2	TIP3	256	87.509	21.566	5.114	1.00	54.21
ATOM	3447	OH2	TIP3	257	21.060	10.052	-9.215	1.00	60.32
ATOM	3450	OH2	TIP3	258	11.827	2.450	27.951	1.00	54.26
ATOM	3453	OH2	TIP3	259	64.788	-0.418	3.563	1.00	50.94

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ATOM	3456	OH2	TIP3	260	71.859	28.473	7.950	1.00	62.81
ATOM	3459	OH2	TIP3	261	25.605	-8.106	27.287	1.00	52.81
ATOM	3462	OH2	TIP3	262	-18.804	10.886	12.628	1.00	55.25
ATOM	3465	OH2	TIP3	263	30.652	11.349	16.201	1.00	50.40
ATOM	3468	OH2	TIP3	264	22.350	-16.098	-2.742	1.00	53.27
ATOM	3471	OH2	TIP3	265	29.720	9.106	18.465	1.00	57.23

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TABLE 2

Atom No.	Atom Type	A.A Type	A.A No.	X	Y	Z	OCC	B
ATOM 1	N	GLU	1464	-13.425	16.769	8.973	1.00	61.21
ATOM 3	CA	GLU	1464	-12.536	16.852	7.821	1.00	59.70
ATOM 4	CB	GLU	1464	-11.383	17.829	8.085	1.00	60.05
ATOM 5	C	GLU	1464	-11.998	15.478	7.427	1.00	57.11
ATOM 6	O	GLU	1464	-12.134	15.076	6.274	1.00	59.75
ATOM 7	N	LEU	1465	-11.406	14.749	8.368	1.00	52.21
ATOM 9	CA	LEU	1465	-10.871	13.424	8.062	1.00	46.72
ATOM 10	CB	LEU	1465	-10.102	12.844	9.249	1.00	44.98
ATOM 11	CG	LEU	1465	-8.608	13.123	9.384	1.00	46.11
ATOM 12	CD1	LEU	1465	-8.338	14.592	9.663	1.00	51.13
ATOM 13	CD2	LEU	1465	-8.064	12.286	10.512	1.00	4.99
ATOM 14	C	LEU	1465	-12.000	12.475	7.700	1.00	44.16
ATOM 15	O	LEU	1465	-13.101	12.577	8.239	1.00	44.04
ATOM 16	N	PRO	1466	-11.760	11.580	6.732	1.00	42.53
ATOM 17	CD	PRO	1466	-10.535	11.534	5.913	1.00	41.30
ATOM 18	CA	PRO	1466	-12.740	10.591	6.269	1.00	41.16
ATOM 19	CB	PRO	1466	-12.134	10.111	4.959	1.00	41.48
ATOM 20	CG	PRO	1466	-10.658	10.213	5.220	1.00	41.30
ATOM 21	C	PRO	1466	-12.906	9.441	7.261	1.00	41.31
ATOM 22	O	PRO	1466	-11.929	8.936	7.816	1.00	41.05
ATOM 23	N	GLU	1467	-14.145	9.044	7.500	1.00	41.02
ATOM 25	CA	GLU	1467	-14.428	7.960	8.427	1.00	42.42
ATOM 26	CB	GLU	1467	-15.931	7.904	8.712	1.00	47.98
ATOM 27	CG	GLU	1467	-16.565	9.238	9.105	1.00	52.79
ATOM 28	CD	GLU	1467	-17.998	9.093	9.606	1.00	54.21
ATOM 29	OE1	GLU	1467	-18.474	7.949	9.741	1.00	58.90
ATOM 30	OE2	GLU	1467	-18.650	10.120	9.879	1.00	55.90
ATOM 31	C	GLU	1467	-13.972	6.628	7.837	1.00	40.93
ATOM 32	O	GLU	1467	-14.061	6.426	6.620	1.00	44.32
ATOM 33	N	ASP	1468	-13.473	5.731	8.689	1.00	35.10
ATOM 35	CA	ASP	1468	-13.024	4.404	8.256	1.00	31.82
ATOM 36	CB	ASP	1468	-11.507	4.358	7.992	1.00	30.65
ATOM 37	CG	ASP	1468	-11.025	3.002	7.440	1.00	29.93
ATOM 38	OD1	ASP	1468	-11.689	1.958	7.603	1.00	29.63
ATOM 39	OD2	ASP	1468	-9.945	2.974	6.835	1.00	33.63
ATOM 40	C	ASP	1468	-13.394	3.441	9.369	1.00	31.81
ATOM 41	O	ASP	1468	-12.618	3.209	10.302	1.00	31.91
ATOM 42	N	PRO	1469	-14.569	2.819	9.247	1.00	29.68
ATOM 43	CD	PRO	1469	-15.482	2.963	8.097	1.00	28.33
ATOM 44	CA	PRO	1469	-15.100	1.863	10.220	1.00	31.80
ATOM 45	CB	PRO	1469	-16.352	1.331	9.510	1.00	32.51
ATOM 46	CG	PRO	1469	-16.783	2.496	8.656	1.00	27.41
ATOM 47	C	PRO	1469	-14.146	0.731	10.590	1.00	30.44
ATOM 48	O	PRO	1469	-14.272	0.135	11.654	1.00	30.02
ATOM 49	N	ARG	1470	-13.198	0.442	9.704	1.00	31.06
ATOM 51	CA	ARG	1470	-12.240	-0.636	9.917	1.00	31.86
ATOM 52	CB	ARG	1470	-11.386	-0.860	8.660	1.00	31.36
ATOM 53	CG	ARG	1470	-12.107	-1.437	7.448	1.00	33.08

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ATOM	54	CD	ARG	1470	-11.148	-1.588	6.248	1.00	31.08
ATOM	55	NE	ARG	1470	-10.540	-0.310	5.891	1.00	34.36
ATOM	57	CZ	ARG	1470	-9.656	-0.135	4.919	1.00	33.32
ATOM	58	NH1	ARG	1470	-9.260	-1.164	4.185	1.00	35.90
ATOM	61	NH2	ARG	1470	-9.155	1.074	4.687	1.00	32.79
ATOM	64	C	ARG	1470	-11.290	-0.436	11.095	1.00	32.68
ATOM	65	O	ARG	1470	-10.820	-1.410	11.683	1.00	33.43
ATOM	66	N	TRP	1471	-11.031	0.814	11.456	1.00	31.84
ATOM	68	CA	TRP	1471	-10.063	1.090	12.505	1.00	31.17
ATOM	69	CB	TRP	1471	-8.816	1.677	11.850	1.00	30.15
ATOM	70	CG	TRP	1471	-8.173	0.725	10.941	1.00	29.54
ATOM	71	CD2	TRP	1471	-7.288	-0.329	11.315	1.00	31.07
ATOM	72	CE2	TRP	1471	-6.913	-0.992	10.132	1.00	34.41
ATOM	73	CE3	TRP	1471	-6.762	-0.768	12.536	1.00	29.46
ATOM	74	CD1	TRP	1471	-8.309	0.660	9.587	1.00	30.20
ATOM	75	NE1	TRP	1471	-7.557	-0.371	9.089	1.00	33.09
ATOM	77	CZ2	TRP	1471	-6.042	-2.085	10.135	1.00	31.68
ATOM	78	CZ3	TRP	1471	-5.897	-1.853	12.540	1.00	29.65
ATOM	79	CH2	TRP	1471	-5.541	-2.494	11.347	1.00	30.18
ATOM	80	C	TRP	1471	-10.477	2.019	13.620	1.00	29.94
ATOM	81	O	TRP	1471	-9.782	2.108	14.631	1.00	30.00
ATOM	82	N	GLU	1472	-11.573	2.737	13.416	1.00	29.06
ATOM	84	CA	GLU	1472	-12.051	3.706	14.380	1.00	28.62
ATOM	85	CB	GLU	1472	-13.312	4.386	13.849	1.00	29.16
ATOM	86	CG	GLU	1472	-13.641	5.733	14.529	1.00	30.74
ATOM	87	CD	GLU	1472	-12.676	6.848	14.156	1.00	30.05
ATOM	88	OE1	GLU	1472	-12.090	6.799	13.057	1.00	31.32
ATOM	89	OE2	GLU	1472	-12.511	7.784	14.961	1.00	30.26
ATOM	90	C	GLU	1472	-12.327	3.159	15.767	1.00	28.70
ATOM	91	O	GLU	1472	-12.969	2.125	15.916	1.00	31.01
ATOM	92	N	LEU	1473	-11.810	3.842	16.781	1.00	27.38
ATOM	94	CA	LEU	1473	-12.054	3.451	18.161	1.00	29.61
ATOM	95	CB	LEU	1473	-10.763	3.073	18.899	1.00	28.56
ATOM	96	CG	LEU	1473	-10.923	2.756	20.403	1.00	30.06
ATOM	97	CD1	LEU	1473	-11.485	1.354	20.639	1.00	28.42
ATOM	98	CD2	LEU	1473	-9.595	2.876	21.115	1.00	28.15
ATOM	99	C	LEU	1473	-12.617	4.714	18.764	1.00	31.81
ATOM	100	O	LEU	1473	-12.179	5.814	18.407	1.00	33.00
ATOM	101	N	PRO	1474	-13.670	4.591	19.596	1.00	31.45
ATOM	102	CD	PRO	1474	-14.488	3.400	19.859	1.00	31.72
ATOM	103	CA	PRO	1474	-14.261	5.774	20.226	1.00	31.23
ATOM	104	CB	PRO	1474	-15.400	5.176	21.048	1.00	29.01
ATOM	105	CG	PRO	1474	-15.815	4.005	20.247	1.00	29.09
ATOM	106	C	PRO	1474	-13.217	6.444	21.120	1.00	33.36
ATOM	107	O	PRO	1474	-12.447	5.765	21.808	1.00	36.40
ATOM	108	N	ARG	1475	-13.188	7.770	21.112	1.00	33.67
ATOM	110	CA	ARG	1475	-12.228	8.498	21.924	1.00	33.96
ATOM	111	CB	ARG	1475	-12.433	9.991	21.735	1.00	35.31
ATOM	112	CG	ARG	1475	-12.134	10.405	20.333	1.00	40.10
ATOM	113	CD	ARG	1475	-12.060	11.906	20.145	1.00	42.98
ATOM	114	NE	ARG	1475	-11.785	12.194	18.737	1.00	42.91
ATOM	116	CZ	ARG	1475	-10.578	12.443	18.253	1.00	41.30
ATOM	117	NH1	ARG	1475	-9.529	12.467	19.064	1.00	41.88
ATOM	120	NH2	ARG	1475	-10.413	12.567	16.943	1.00	40.98

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ATOM	123	C	ARG	1475	-12.278	8.142	23.404	1.00	35.88
ATOM	124	O	ARG	1475	-11.240	8.046	24.061	1.00	37.10
ATOM	125	N	ASP	1476	-13.479	7.920	23.928	1.00	36.47
ATOM	127	CA	ASP	1476	-13.632	7.581	25.335	1.00	37.24
ATOM	128	CB	ASP	1476	-15.112	7.629	25.741	1.00	39.66
ATOM	129	CG	ASP	1476	-15.930	6.480	25.163	1.00	42.38
ATOM	130	OD1	ASP	1476	-15.438	5.706	24.322	1.00	47.52
ATOM	131	OD2	ASP	1476	-17.098	6.349	25.568	1.00	48.06
ATOM	132	C	ASP	1476	-13.023	6.232	25.724	1.00	36.93
ATOM	133	O	ASP	1476	-13.034	5.856	26.898	1.00	40.09
ATOM	134	N	ARG	1477	-12.564	5.475	24.732	1.00	34.34
ATOM	136	CA	ARG	1477	-11.961	4.171	24.993	1.00	32.47
ATOM	137	CB	ARG	1477	-12.269	3.212	23.852	1.00	31.59
ATOM	138	CG	ARG	1477	-13.716	2.939	23.640	1.00	29.66
ATOM	139	CD	ARG	1477	-14.314	2.342	24.875	1.00	30.65
ATOM	140	NE	ARG	1477	-14.498	3.342	25.918	1.00	31.37
ATOM	142	CZ	ARG	1477	-14.822	3.055	27.174	1.00	32.81
ATOM	143	NH1	ARG	1477	-15.002	1.794	27.549	1.00	33.92
ATOM	146	NH2	ARG	1477	-14.950	4.025	28.062	1.00	31.74
ATOM	149	C	ARG	1477	-10.452	4.266	25.153	1.00	33.13
ATOM	150	O	ARG	1477	-9.777	3.281	25.445	1.00	33.55
ATOM	151	N	LEU	1478	-9.923	5.466	24.984	1.00	34.43
ATOM	153	CA	LEU	1478	-8.493	5.663	25.076	1.00	35.68
ATOM	154	CB	LEU	1478	-8.008	6.350	23.790	1.00	34.98
ATOM	155	CG	LEU	1478	-6.581	6.137	23.284	1.00	31.11
ATOM	156	CD1	LEU	1478	-6.280	4.650	23.161	1.00	26.62
ATOM	157	CD2	LEU	1478	-6.428	6.839	21.940	1.00	28.80
ATOM	158	C	LEU	1478	-8.158	6.505	26.295	1.00	36.21
ATOM	159	O	LEU	1478	-8.501	7.688	26.361	1.00	39.67
ATOM	160	N	VAL	1479	-7.558	5.878	27.293	1.00	35.42
ATOM	162	CA	VAL	1479	-7.156	6.599	28.491	1.00	35.80
ATOM	163	CB	VAL	1479	-7.269	5.707	29.742	1.00	36.29
ATOM	164	CG1	VAL	1479	-7.017	6.527	30.983	1.00	37.23
ATOM	165	CG2	VAL	1479	-8.650	5.059	29.812	1.00	34.41
ATOM	166	C	VAL	1479	-5.704	7.046	28.244	1.00	35.68
ATOM	167	O	VAL	1479	-4.764	6.246	28.319	1.00	33.45
ATOM	168	N	LEU	1480	-5.538	8.315	27.885	1.00	38.15
ATOM	170	CA	LEU	1480	-4.213	8.860	27.584	1.00	42.61
ATOM	171	CB	LEU	1480	-4.332	10.205	26.857	1.00	39.14
ATOM	172	CG	LEU	1480	-4.969	10.179	25.460	1.00	38.44
ATOM	173	CD1	LEU	1480	-4.901	11.579	24.879	1.00	39.39
ATOM	174	CD2	LEU	1480	-4.263	9.194	24.533	1.00	36.86
ATOM	175	C	LEU	1480	-3.274	8.970	28.783	1.00	46.37
ATOM	176	O	LEU	1480	-3.659	9.445	29.850	1.00	48.86
ATOM	177	N	GLY	1481	-2.033	8.537	28.594	1.00	47.13
ATOM	179	CA	GLY	1481	-1.081	8.573	29.678	1.00	48.19
ATOM	180	C	GLY	1481	0.163	9.388	29.425	1.00	50.27
ATOM	181	O	GLY	1481	0.152	10.367	28.675	1.00	51.19
ATOM	182	N	LYS	1482	1.240	8.965	30.078	1.00	50.93
ATOM	184	CA	LYS	1482	2.543	9.606	30.007	1.00	50.94
ATOM	185	CB	LYS	1482	3.509	8.866	30.933	1.00	50.41
ATOM	186	CG	LYS	1482	4.971	9.026	30.567	1.00	51.87
ATOM	187	CD	LYS	1482	5.810	7.874	31.087	1.00	53.49
ATOM	188	CE	LYS	1482	5.390	6.542	30.478	1.00	50.77

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ATOM	189	NZ	LYS	1482	6.251	5.433	30.986	1.00	49.92
ATOM	193	C	LYS	1482	3.145	9.676	28.609	1.00	52.31
ATOM	194	O	LYS	1482	3.115	8.700	27.851	1.00	52.30
ATOM	195	N	PRO	1483	3.706	10.838	28.250	1.00	53.47
ATOM	196	CD	PRO	1483	3.667	12.105	28.997	1.00	54.19
ATOM	197	CA	PRO	1483	4.326	11.021	26.937	1.00	54.10
ATOM	198	CB	PRO	1483	4.772	12.480	26.976	1.00	54.25
ATOM	199	CG	PRO	1483	3.772	13.118	27.895	1.00	55.30
ATOM	200	C	PRO	1483	5.535	10.096	26.827	1.00	54.72
ATOM	201	O	PRO	1483	6.343	10.017	27.751	1.00	53.48
ATOM	202	N	LEU	1484	5.619	9.351	25.731	1.00	57.05
ATOM	204	CA	LEU	1484	6.739	8.447	25.503	1.00	59.26
ATOM	205	CB	LEU	1484	6.307	7.241	24.669	1.00	59.35
ATOM	206	CG	LEU	1484	5.391	6.216	25.343	1.00	60.87
ATOM	207	CD1	LEU	1484	4.975	5.161	24.329	1.00	57.14
ATOM	208	CD2	LEU	1484	6.081	5.571	26.551	1.00	59.79
ATOM	209	C	LEU	1484	7.847	9.194	24.778	1.00	61.30
ATOM	210	O	LEU	1484	8.980	8.720	24.701	1.00	62.17
ATOM	211	N	GLY	1485	7.494	10.351	24.220	1.00	63.75
ATOM	213	CA	GLY	1485	8.456	11.173	23.507	1.00	66.33
ATOM	214	C	GLY	1485	8.081	11.412	22.054	1.00	67.79
ATOM	215	O	GLY	1485	6.918	11.653	21.727	1.00	69.61
ATOM	216	N	GLN	1491	4.615	13.762	18.385	1.00	58.26
ATOM	218	CA	GLN	1491	4.353	13.353	19.762	1.00	57.98
ATOM	219	CB	GLN	1491	3.476	14.379	20.468	1.00	61.80
ATOM	220	CG	GLN	1491	3.134	14.034	21.920	1.00	70.31
ATOM	221	CD	GLN	1491	2.019	14.911	22.482	1.00	75.91
ATOM	222	OE1	GLN	1491	1.355	15.636	21.748	1.00	77.85
ATOM	223	NE2	GLN	1491	1.820	14.832	23.788	1.00	78.30
ATOM	226	C	GLN	1491	3.709	11.965	19.881	1.00	54.67
ATOM	227	O	GLN	1491	2.701	11.669	19.222	1.00	54.91
ATOM	228	N	VAL	1492	4.305	11.125	20.729	1.00	50.04
ATOM	230	CA	VAL	1492	3.825	9.763	20.988	1.00	44.93
ATOM	231	CB	VAL	1492	4.861	8.705	20.583	1.00	42.65
ATOM	232	CG1	VAL	1492	4.378	7.325	20.958	1.00	39.71
ATOM	233	CG2	VAL	1492	5.119	8.766	19.099	1.00	40.98
ATOM	234	C	VAL	1492	3.584	9.661	22.490	1.00	43.43
ATOM	235	O	VAL	1492	4.451	10.029	23.289	1.00	43.43
ATOM	236	N	VAL	1493	2.400	9.212	22.888	1.00	41.13
ATOM	238	CA	VAL	1493	2.107	9.080	24.304	1.00	38.77
ATOM	239	CB	VAL	1493	1.052	10.133	24.782	1.00	36.35
ATOM	240	CG1	VAL	1493	1.410	11.508	24.287	1.00	36.06
ATOM	241	CG2	VAL	1493	-0.329	9.755	24.339	1.00	37.64
ATOM	242	C	VAL	1493	1.589	7.693	24.619	1.00	37.77
ATOM	243	O	VAL	1493	0.948	7.058	23.783	1.00	38.88
ATOM	244	N	LEU	1494	1.949	7.187	25.790	1.00	36.24
ATOM	246	CA	LEU	1494	1.468	5.880	26.205	1.00	35.92
ATOM	247	CB	LEU	1494	2.252	5.383	27.429	1.00	35.41
ATOM	248	CG	LEU	1494	1.886	4.009	28.004	1.00	36.21
ATOM	249	CD1	LEU	1494	1.927	2.931	26.924	1.00	33.60
ATOM	250	CD2	LEU	1494	2.835	3.670	29.145	1.00	36.03
ATOM	251	C	LEU	1494	-0.010	6.095	26.564	1.00	35.27
ATOM	252	O	LEU	1494	-0.425	7.215	26.887	1.00	34.35
ATOM	253	N	ALA	1495	-0.807	5.043	26.468	1.00	34.93

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ATOM	255	CA	ALA	1495	-2.220	5.145	26.768	1.00	34.44
ATOM	256	CB	ALA	1495	-2.955	5.794	25.616	1.00	35.29
ATOM	257	C	ALA	1495	-2.781	3.770	27.018	1.00	34.59
ATOM	258	O	ALA	1495	-2.128	2.766	26.748	1.00	35.52
ATOM	259	N	GLU	1496	-3.996	3.723	27.536	1.00	36.64
ATOM	261	CA	GLU	1496	-4.652	2.462	27.806	1.00	37.57
ATOM	262	CB	GLU	1496	-5.000	2.354	29.287	1.00	38.97
ATOM	263	CG	GLU	1496	-3.769	2.304	30.185	1.00	41.79
ATOM	264	CD	GLU	1496	-4.110	2.475	31.645	1.00	43.65
ATOM	265	OE1	GLU	1496	-4.408	3.617	32.036	1.00	42.97
ATOM	266	OE2	GLU	1496	-4.086	1.475	32.398	1.00	46.65
ATOM	267	C	GLU	1496	-5.896	2.404	26.943	1.00	38.50
ATOM	268	O	GLU	1496	-6.660	3.371	26.867	1.00	40.28
ATOM	269	N	ALA	1497	-6.051	1.301	26.223	1.00	37.34
ATOM	271	CA	ALA	1497	-7.194	1.131	25.352	1.00	37.42
ATOM	272	CB	ALA	1497	-6.743	0.625	23.985	1.00	35.92
ATOM	273	C	ALA	1497	-8.146	0.148	26.000	1.00	36.77
ATOM	274	O	ALA	1497	-7.759	-0.977	26.323	1.00	35.74
ATOM	275	N	ILE	1498	-9.354	0.616	26.291	1.00	37.03
ATOM	277	CA	ILE	1498	-10.378	-0.224	26.896	1.00	36.80
ATOM	278	CB	ILE	1498	-11.372	0.612	27.728	1.00	34.53
ATOM	279	CG2	ILE	1498	-12.373	-0.290	28.425	1.00	34.59
ATOM	280	CG1	ILE	1498	-10.640	1.438	28.778	1.00	31.97
ATOM	281	CD1	ILE	1498	-11.552	2.344	29.541	1.00	31.12
ATOM	282	C	ILE	1498	-11.126	-0.807	25.709	1.00	38.72
ATOM	283	O	ILE	1498	-11.647	-0.066	24.879	1.00	37.74
ATOM	284	N	GLY	1499	-11.137	-2.126	25.590	1.00	40.98
ATOM	286	CA	GLY	1499	-11.839	-2.728	24.482	1.00	44.64
ATOM	287	C	GLY	1499	-10.931	-3.115	23.332	1.00	48.45
ATOM	288	O	GLY	1499	-10.260	-4.147	23.401	1.00	51.92
ATOM	289	N	LEU	1500	-10.877	-2.269	22.303	1.00	47.87
ATOM	291	CA	LEU	1500	-10.076	-2.530	21.102	1.00	46.80
ATOM	292	CB	LEU	1500	-8.594	-2.770	21.434	1.00	45.37
ATOM	293	CG	LEU	1500	-7.543	-1.661	21.293	1.00	44.84
ATOM	294	CD1	LEU	1500	-6.174	-2.290	21.450	1.00	43.33
ATOM	295	CD2	LEU	1500	-7.623	-0.959	19.948	1.00	40.43
ATOM	296	C	LEU	1500	-10.631	-3.737	20.349	1.00	45.63
ATOM	297	O	LEU	1500	-10.797	-4.823	20.915	1.00	44.42
ATOM	298	N	PRO	1505	-13.569	-5.910	25.549	1.00	52.13
ATOM	299	CD	PRO	1505	-14.316	-7.170	25.398	1.00	54.09
ATOM	300	CA	PRO	1505	-14.451	-4.828	25.999	1.00	50.46
ATOM	301	CB	PRO	1505	-15.841	-5.455	25.891	1.00	49.86
ATOM	302	CG	PRO	1505	-15.586	-6.898	26.193	1.00	52.17
ATOM	303	C	PRO	1505	-14.136	-4.370	27.422	1.00	47.75
ATOM	304	O	PRO	1505	-14.148	-3.180	27.710	1.00	47.93
ATOM	305	N	ASN	1506	-13.778	-5.313	28.285	1.00	46.20
ATOM	307	CA	ASN	1506	-13.458	-4.986	29.666	1.00	49.52
ATOM	308	CB	ASN	1506	-14.310	-5.829	30.612	1.00	52.42
ATOM	309	CG	ASN	1506	-15.788	-5.489	30.526	1.00	54.50
ATOM	310	OD1	ASN	1506	-16.179	-4.331	30.680	1.00	57.16
ATOM	311	ND2	ASN	1506	-16.610	-6.489	30.244	1.00	56.82
ATOM	314	C	ASN	1506	-11.973	-5.124	30.003	1.00	50.65
ATOM	315	O	ASN	1506	-11.583	-5.174	31.178	1.00	50.65
ATOM	316	N	ARG	1507	-11.142	-5.145	28.968	1.00	50.90

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ATOM	318	CA	ARG	1507	-9.700	-5.276	29.127	1.00	49.77
ATOM	319	CB	ARG	1507	-9.192	-6.483	28.339	1.00	55.81
ATOM	320	CG	ARG	1507	-9.450	-7.833	28.988	1.00	61.63
ATOM	321	CD	ARG	1507	-8.408	-8.149	30.041	1.00	66.01
ATOM	322	NE	ARG	1507	-8.600	-9.490	30.583	1.00	72.55
ATOM	324	CZ	ARG	1507	-8.024	-9.944	31.694	1.00	77.32
ATOM	325	NH1	ARG	1507	-7.198	-9.169	32.392	1.00	78.41
ATOM	328	NH2	ARG	1507	-8.335	-11.151	32.147	1.00	79.30
ATOM	331	C	ARG	1507	-9.015	-4.036	28.595	1.00	45.60
ATOM	332	O	ARG	1507	-9.452	-3.464	27.590	1.00	42.08
ATOM	333	N	VAL	1508	-7.977	-3.597	29.297	1.00	42.86
ATOM	335	CA	VAL	1508	-7.216	-2.443	28.858	1.00	40.75
ATOM	336	CB	VAL	1508	-6.903	-1.428	30.010	1.00	38.75
ATOM	337	CG1	VAL	1508	-8.184	-1.015	30.702	1.00	43.29
ATOM	338	CG2	VAL	1508	-5.919	-2.005	31.012	1.00	37.56
ATOM	339	C	VAL	1508	-5.929	-2.970	28.248	1.00	39.14
ATOM	340	O	VAL	1508	-5.369	-3.972	28.708	1.00	39.16
ATOM	341	N	THR	1509	-5.517	-2.345	27.157	1.00	37.26
ATOM	343	CA	THR	1509	-4.298	-2.737	26.486	1.00	36.52
ATOM	344	CB	THR	1509	-4.571	-3.187	25.019	1.00	37.83
ATOM	345	OG1	THR	1509	-5.423	-4.340	25.011	1.00	43.88
ATOM	347	CG2	THR	1509	-3.267	-3.540	24.310	1.00	34.51
ATOM	348	C	THR	1509	-3.434	-1.495	26.473	1.00	35.82
ATOM	349	O	THR	1509	-3.927	-0.408	26.174	1.00	34.37
ATOM	350	N	LYS	1510	-2.175	-1.628	26.880	1.00	35.96
ATOM	352	CA	LYS	1510	-1.291	-0.479	26.843	1.00	36.13
ATOM	353	CB	LYS	1510	-0.032	-0.695	27.680	1.00	37.77
ATOM	354	CG	LYS	1510	-0.277	-0.854	29.162	1.00	44.58
ATOM	355	CD	LYS	1510	1.023	-0.658	29.948	1.00	51.33
ATOM	356	CE	LYS	1510	0.947	-1.286	31.342	1.00	58.15
ATOM	357	NZ	LYS	1510	-0.149	-0.728	32.187	1.00	64.94
ATOM	361	C	LYS	1510	-0.929	-0.355	25.373	1.00	34.59
ATOM	362	O	LYS	1510	-0.574	-1.345	24.734	1.00	31.43
ATOM	363	N	VAL	1511	-1.092	0.846	24.835	1.00	32.95
ATOM	365	CA	VAL	1511	-0.810	1.121	23.441	1.00	32.29
ATOM	366	CB	VAL	1511	-2.129	1.213	22.621	1.00	32.95
ATOM	367	CG1	VAL	1511	-2.879	-0.109	22.686	1.00	34.79
ATOM	368	CG2	VAL	1511	-3.026	2.354	23.148	1.00	32.84
ATOM	369	C	VAL	1511	-0.058	2.446	23.353	1.00	32.65
ATOM	370	O	VAL	1511	0.021	3.185	24.344	1.00	31.62
ATOM	371	N	ALA	1512	0.521	2.721	22.186	1.00	30.24
ATOM	373	CA	ALA	1512	1.244	3.969	21.954	1.00	28.18
ATOM	374	CB	ALA	1512	2.599	3.700	21.316	1.00	25.62
ATOM	375	C	ALA	1512	0.373	4.783	21.015	1.00	27.54
ATOM	376	O	ALA	1512	-0.151	4.264	20.040	1.00	27.17
ATOM	377	N	VAL	1513	0.204	6.054	21.322	1.00	30.52
ATOM	379	CA	VAL	1513	-0.630	6.914	20.503	1.00	34.08
ATOM	380	CB	VAL	1513	-1.731	7.591	21.347	1.00	34.61
ATOM	381	CG1	VAL	1513	-2.607	8.444	20.474	1.00	36.75
ATOM	382	CG2	VAL	1513	-2.567	6.549	22.087	1.00	33.45
ATOM	383	C	VAL	1513	0.203	8.008	19.837	1.00	36.38
ATOM	384	O	VAL	1513	0.924	8.750	20.510	1.00	35.32
ATOM	385	N	LYS	1514	0.105	8.093	18.513	1.00	38.19
ATOM	387	CA	LYS	1514	0.818	9.104	17.746	1.00	40.12

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ATOM	388	CB	LYS	1514	1.339	8.513	16.439	1.00	40.93
ATOM	389	CG	LYS	1514	2.452	7.488	16.632	1.00	42.52
ATOM	390	CD	LYS	1514	2.861	6.803	15.338	1.00	46.25
ATOM	391	CE	LYS	1514	3.268	7.796	14.261	1.00	49.76
ATOM	392	NZ	LYS	1514	4.304	8.771	14.705	1.00	52.14
ATOM	396	C	LYS	1514	-0.166	10.215	17.458	1.00	40.69
ATOM	397	O	LYS	1514	-1.313	9.953	17.110	1.00	41.69
ATOM	398	N	MET	1515	0.277	11.454	17.613	1.00	43.28
ATOM	400	CA	MET	1515	-0.569	12.610	17.379	1.00	46.21
ATOM	401	CB	MET	1515	-1.363	12.936	18.644	1.00	46.96
ATOM	402	CG	MET	1515	-0.488	13.293	19.837	1.00	47.61
ATOM	403	SD	MET	1515	-1.413	13.464	21.358	1.00	49.77
ATOM	404	CE	MET	1515	-1.593	11.761	21.814	1.00	47.84
ATOM	405	C	MET	1515	0.299	13.805	17.000	1.00	49.90
ATOM	406	O	MET	1515	1.519	13.788	17.194	1.00	49.83
ATOM	407	N	LEU	1516	-0.339	14.822	16.430	1.00	54.45
ATOM	409	CA	LEU	1516	0.335	16.053	16.023	1.00	57.57
ATOM	410	CB	LEU	1516	-0.483	16.762	14.944	1.00	54.10
ATOM	411	CG	LEU	1516	-0.800	16.007	13.664	1.00	50.71
ATOM	412	CD1	LEU	1516	-1.830	16.800	12.901	1.00	51.20
ATOM	413	CD2	LEU	1516	0.467	15.809	12.849	1.00	50.08
ATOM	414	C	LEU	1516	0.487	17.010	17.202	1.00	61.88
ATOM	415	O	LEU	1516	-0.170	16.852	18.235	1.00	63.30
ATOM	416	N	LYS	1517	1.335	18.018	17.021	1.00	66.83
ATOM	418	CA	LYS	1517	1.568	19.036	18.037	1.00	71.46
ATOM	419	CB	LYS	1517	2.985	19.593	17.911	1.00	76.28
ATOM	420	CG	LYS	1517	4.084	18.626	18.349	1.00	82.19
ATOM	421	CD	LYS	1517	5.450	19.085	17.846	1.00	86.93
ATOM	422	CE	LYS	1517	6.579	18.228	18.411	1.00	90.46
ATOM	423	NZ	LYS	1517	7.896	18.513	17.763	1.00	92.51
ATOM	427	C	LYS	1517	0.549	20.156	17.837	1.00	72.44
ATOM	428	O	LYS	1517	-0.142	20.198	16.819	1.00	72.12
ATOM	429	N	SER	1518	0.474	21.075	18.793	1.00	73.90
ATOM	431	CA	SER	1518	-0.470	22.185	18.697	1.00	74.96
ATOM	432	CB	SER	1518	-0.498	22.980	20.002	1.00	74.72
ATOM	433	C	SER	1518	-0.133	23.100	17.525	1.00	76.16
ATOM	434	O	SER	1518	-1.029	23.667	16.897	1.00	76.56
ATOM	435	N	ASP	1519	1.158	23.245	17.232	1.00	77.24
ATOM	437	CA	ASP	1519	1.601	24.094	16.125	1.00	78.51
ATOM	438	CB	ASP	1519	2.849	24.888	16.535	1.00	79.70
ATOM	439	C	ASP	1519	1.887	23.264	14.865	1.00	78.29
ATOM	440	O	ASP	1519	2.797	23.580	14.088	1.00	78.52
ATOM	441	N	ALA	1520	1.121	22.192	14.682	1.00	76.90
ATOM	443	CA	ALA	1520	1.285	21.313	13.529	1.00	74.09
ATOM	444	CB	ALA	1520	0.737	19.930	13.840	1.00	74.20
ATOM	445	C	ALA	1520	0.580	21.895	12.318	1.00	71.82
ATOM	446	O	ALA	1520	-0.573	22.311	12.400	1.00	71.78
ATOM	447	N	THR	1521	1.291	21.951	11.202	1.00	69.97
ATOM	449	CA	THR	1521	0.734	22.480	9.970	1.00	68.86
ATOM	450	CB	THR	1521	1.848	22.911	9.026	1.00	68.87
ATOM	451	OG1	THR	1521	2.621	21.762	8.651	1.00	70.03
ATOM	453	CG2	THR	1521	2.756	23.912	9.715	1.00	71.55
ATOM	454	C	THR	1521	-0.081	21.389	9.292	1.00	67.89
ATOM	455	O	THR	1521	0.111	20.204	9.563	1.00	69.03

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ATOM	456	N	GLU	1522	-0.964	21.783	8.382	1.00	66.59
ATOM	458	CA	GLU	1522	-1.785	20.821	7.657	1.00	65.71
ATOM	459	CB	GLU	1522	-2.737	21.532	6.692	1.00	65.61
ATOM	460	C	GLU	1522	-0.886	19.823	6.909	1.00	64.32
ATOM	461	O	GLU	1522	-1.324	18.729	6.549	1.00	66.29
ATOM	462	N	LYS	1523	0.367	20.205	6.677	1.00	59.93
ATOM	464	CA	LYS	1523	1.314	19.326	6.016	1.00	57.38
ATOM	465	CB	LYS	1523	2.629	20.064	5.747	1.00	60.47
ATOM	466	CG	LYS	1523	3.815	19.162	5.370	1.00	62.75
ATOM	467	CD	LYS	1523	3.510	18.288	4.160	1.00	63.95
ATOM	468	CE	LYS	1523	4.759	17.596	3.652	1.00	65.88
ATOM	469	NZ	LYS	1523	4.429	16.721	2.494	1.00	70.37
ATOM	473	C	LYS	1523	1.565	18.173	6.974	1.00	54.80
ATOM	474	O	LYS	1523	1.548	17.003	6.581	1.00	54.44
ATOM	475	N	ASP	1524	1.786	18.523	8.239	1.00	51.67
ATOM	477	CA	ASP	1524	2.036	17.549	9.295	1.00	49.43
ATOM	478	CB	ASP	1524	2.297	18.271	10.622	1.00	51.06
ATOM	479	CG	ASP	1524	3.598	19.080	10.613	1.00	54.03
ATOM	480	OD1	ASP	1524	3.649	20.136	11.283	1.00	56.32
ATOM	481	OD2	ASP	1524	4.580	18.658	9.956	1.00	56.02
ATOM	482	C	ASP	1524	0.847	16.596	9.413	1.00	47.73
ATOM	483	O	ASP	1524	1.017	15.387	9.580	1.00	45.85
ATOM	484	N	LEU	1525	-0.354	17.155	9.300	1.00	47.62
ATOM	486	CA	LEU	1525	-1.585	16.380	9.354	1.00	45.95
ATOM	487	CB	LEU	1525	-2.801	17.307	9.271	1.00	43.61
ATOM	488	CG	LEU	1525	-4.193	16.665	9.234	1.00	44.56
ATOM	489	CD1	LEU	1525	-4.364	15.543	10.268	1.00	46.02
ATOM	490	CD2	LEU	1525	-5.215	17.740	9.468	1.00	43.80
ATOM	491	C	LEU	1525	-1.605	15.372	8.210	1.00	45.67
ATOM	492	O	LEU	1525	-1.921	14.204	8.416	1.00	46.78
ATOM	493	N	SER	1526	-1.245	15.822	7.014	1.00	45.44
ATOM	495	CA	SER	1526	-1.211	14.945	5.851	1.00	46.33
ATOM	496	CB	SER	1526	-0.903	15.744	4.584	1.00	48.48
ATOM	497	OG	SER	1526	-2.012	16.546	4.218	1.00	57.28
ATOM	499	C	SER	1526	-0.192	13.821	5.995	1.00	43.84
ATOM	500	O	SER	1526	-0.480	12.669	5.674	1.00	45.24
ATOM	501	N	ASP	1527	0.994	14.144	6.489	1.00	40.88
ATOM	503	CA	ASP	1527	2.024	13.128	6.646	1.00	39.70
ATOM	504	CB	ASP	1527	3.376	13.767	6.960	1.00	37.62
ATOM	505	CG	ASP	1527	3.934	14.555	5.786	1.00	37.01
ATOM	506	OD1	ASP	1527	3.399	14.434	4.657	1.00	35.78
ATOM	507	OD2	ASP	1527	4.916	15.295	5.992	1.00	40.23
ATOM	508	C	ASP	1527	1.652	12.053	7.659	1.00	38.51
ATOM	509	O	ASP	1527	1.951	10.872	7.461	1.00	37.68
ATOM	510	N	LEU	1528	0.973	12.460	8.725	1.00	38.16
ATOM	512	CA	LEU	1528	0.532	11.513	9.744	1.00	38.29
ATOM	513	CB	LEU	1528	0.026	12.258	10.985	1.00	37.12
ATOM	514	CG	LEU	1528	-0.505	11.412	12.153	1.00	39.03
ATOM	515	CD1	LEU	1528	0.499	10.323	12.539	1.00	35.39
ATOM	516	CD2	LEU	1528	-0.825	12.315	13.334	1.00	35.29
ATOM	517	C	LEU	1528	-0.568	10.611	9.155	1.00	38.10
ATOM	518	O	LEU	1528	-0.607	9.400	9.413	1.00	37.21
ATOM	519	N	ILE	1529	-1.450	11.210	8.355	1.00	36.71
ATOM	521	CA	ILE	1529	-2.531	10.472	7.718	1.00	35.93

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ATOM	522	CB	ILE	1529	-3.486	11.419	6.931	1.00	35.67
ATOM	523	CG2	ILE	1529	-4.492	10.619	6.119	1.00	34.04
ATOM	524	CG1	ILE	1529	-4.259	12.295	7.916	1.00	33.81
ATOM	525	CD1	ILE	1529	-5.177	13.288	7.276	1.00	33.58
ATOM	526	C	ILE	1529	-1.912	9.447	6.786	1.00	37.49
ATOM	527	O	ILE	1529	-2.274	8.269	6.829	1.00	37.11
ATOM	528	N	SER	1530	-0.926	9.893	6.003	1.00	38.20
ATOM	530	CA	SER	1530	-0.217	9.036	5.050	1.00	37.49
ATOM	531	CB	SER	1530	0.911	9.822	4.370	1.00	43.32
ATOM	532	OG	SER	1530	0.424	10.970	3.687	1.00	52.31
ATOM	534	C	SER	1530	0.382	7.808	5.719	1.00	34.40
ATOM	535	O	SER	1530	0.234	6.691	5.219	1.00	31.51
ATOM	536	N	GLU	1531	1.048	8.028	6.851	1.00	32.08
ATOM	538	CA	GLU	1531	1.690	6.952	7.594	1.00	30.60
ATOM	539	CB	GLU	1531	2.506	7.515	8.759	1.00	29.70
ATOM	540	CG	GLU	1531	3.094	6.428	9.657	1.00	30.53
ATOM	541	CD	GLU	1531	3.871	6.962	10.839	1.00	33.17
ATOM	542	OE1	GLU	1531	4.473	6.134	11.552	1.00	33.38
ATOM	543	OE2	GLU	1531	3.883	8.193	11.062	1.00	37.52
ATOM	544	C	GLU	1531	0.698	5.911	8.094	1.00	30.17
ATOM	545	O	GLU	1531	0.991	4.714	8.100	1.00	29.76
ATOM	546	N	MET	1532	-0.464	6.379	8.530	1.00	31.34
ATOM	548	CA	MET	1532	-1.521	5.496	9.015	1.00	30.72
ATOM	549	CB	MET	1532	-2.666	6.336	9.591	1.00	29.99
ATOM	550	CG	MET	1532	-3.880	5.523	10.020	1.00	30.10
ATOM	551	SD	MET	1532	-5.173	6.510	10.727	1.00	29.46
ATOM	552	CE	MET	1532	-5.462	7.682	9.455	1.00	23.76
ATOM	553	C	MET	1532	-2.025	4.638	7.843	1.00	30.47
ATOM	554	O	MET	1532	-2.080	3.401	7.925	1.00	27.05
ATOM	555	N	GLU	1533	-2.387	5.319	6.756	1.00	30.56
ATOM	557	CA	GLU	1533	-2.863	4.674	5.542	1.00	30.56
ATOM	558	CB	GLU	1533	-3.090	5.725	4.458	1.00	28.60
ATOM	559	CG	GLU	1533	-4.226	6.677	4.761	1.00	29.08
ATOM	560	CD	GLU	1533	-5.531	5.954	5.014	1.00	31.28
ATOM	561	OE1	GLU	1533	-6.006	5.230	4.117	1.00	33.09
ATOM	562	OE2	GLU	1533	-6.086	6.104	6.121	1.00	34.97
ATOM	563	C	GLU	1533	-1.861	3.638	5.064	1.00	29.86
ATOM	564	O	GLU	1533	-2.232	2.541	4.677	1.00	32.28
ATOM	565	N	MET	1534	-0.590	4.014	5.107	1.00	32.54
ATOM	567	CA	MET	1534	0.515	3.145	4.719	1.00	33.39
ATOM	568	CB	MET	1534	1.826	3.894	4.885	1.00	34.70
ATOM	569	CG	MET	1534	3.038	3.047	4.654	1.00	44.51
ATOM	570	SD	MET	1534	3.479	3.063	2.943	1.00	52.81
ATOM	571	CE	MET	1534	4.349	4.607	2.874	1.00	47.34
ATOM	572	C	MET	1534	0.530	1.896	5.607	1.00	32.98
ATOM	573	O	MET	1534	0.689	0.776	5.115	1.00	34.00
ATOM	574	N	MET	1535	0.364	2.100	6.910	1.00	31.92
ATOM	576	CA	MET	1535	0.336	0.986	7.848	1.00	30.80
ATOM	577	CB	MET	1535	0.252	1.503	9.294	1.00	33.77
ATOM	578	CG	MET	1535	1.509	2.216	9.810	1.00	32.26
ATOM	579	SD	MET	1535	1.520	2.433	11.617	1.00	34.75
ATOM	580	CE	MET	1535	1.183	4.173	11.723	1.00	37.86
ATOM	581	C	MET	1535	-0.837	0.052	7.521	1.00	30.80
ATOM	582	O	MET	1535	-0.704	-1.175	7.589	1.00	32.03

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ATOM	583	N	LYS	1536	-1.974	0.638	7.142	1.00	31.04
ATOM	585	CA	LYS	1536	-3.170	-0.123	6.767	1.00	31.15
ATOM	586	CB	LYS	1536	-4.334	0.808	6.415	1.00	31.21
ATOM	587	CG	LYS	1536	-4.864	1.625	7.552	1.00	27.76
ATOM	588	CD	LYS	1536	-5.973	2.540	7.103	1.00	21.44
ATOM	589	CE	LYS	1536	-6.434	3.401	8.248	1.00	24.69
ATOM	590	NZ	LYS	1536	-7.578	4.241	7.868	1.00	25.84
ATOM	594	C	LYS	1536	-2.887	-1.003	5.561	1.00	30.71
ATOM	595	O	LYS	1536	-3.238	-2.175	5.560	1.00	34.73
ATOM	596	N	MET	1537	-2.309	-0.412	4.523	1.00	31.18
ATOM	598	CA	MET	1537	-1.967	-1.148	3.307	1.00	31.53
ATOM	599	CB	MET	1537	-1.370	-0.200	2.267	1.00	35.11
ATOM	600	CG	MET	1537	-2.377	0.780	1.654	1.00	42.40
ATOM	601	SD	MET	1537	-3.657	-0.051	0.685	1.00	50.10
ATOM	602	CE	MET	1537	-3.069	0.266	-0.972	1.00	50.20
ATOM	603	C	MET	1537	-0.976	-2.276	3.572	1.00	30.86
ATOM	604	O	MET	1537	-1.218	-3.425	3.210	1.00	30.07
ATOM	605	N	ILE	1538	0.119	-1.950	4.259	1.00	30.92
ATOM	607	CA	ILE	1538	1.173	-2.923	4.563	1.00	28.12
ATOM	608	CB	ILE	1538	2.359	-2.254	5.313	1.00	28.71
ATOM	609	CG2	ILE	1538	3.310	-3.303	5.865	1.00	29.72
ATOM	610	CG1	ILE	1538	3.126	-1.343	4.350	1.00	30.79
ATOM	611	CD1	ILE	1538	4.375	-0.745	4.945	1.00	32.46
ATOM	612	C	ILE	1538	0.717	-4.179	5.299	1.00	26.33
ATOM	613	O	ILE	1538	1.178	-5.276	4.996	1.00	24.20
ATOM	614	N	GLY	1539	-0.188	-4.027	6.258	1.00	27.41
ATOM	616	CA	GLY	1539	-0.651	-5.190	6.997	1.00	27.83
ATOM	617	C	GLY	1539	0.240	-5.533	8.179	1.00	29.10
ATOM	618	O	GLY	1539	1.308	-4.937	8.368	1.00	30.33
ATOM	619	N	LYS	1540	-0.157	-6.561	8.916	1.00	29.46
ATOM	621	CA	LYS	1540	0.539	-6.976	10.120	1.00	29.27
ATOM	622	CB	LYS	1540	-0.470	-7.520	11.139	1.00	27.01
ATOM	623	CG	LYS	1540	-1.438	-6.483	11.638	1.00	29.58
ATOM	624	CD	LYS	1540	-2.496	-7.103	12.530	1.00	39.41
ATOM	625	CE	LYS	1540	-3.548	-6.069	12.952	1.00	44.14
ATOM	626	NZ	LYS	1540	-2.994	-4.996	13.828	1.00	46.92
ATOM	630	C	LYS	1540	1.679	-7.962	10.020	1.00	27.17
ATOM	631	O	LYS	1540	1.745	-8.794	9.111	1.00	26.20
ATOM	632	N	HIS	1541	2.565	-7.856	11.006	1.00	26.96
ATOM	634	CA	HIS	1541	3.690	-8.761	11.144	1.00	27.30
ATOM	635	CB	HIS	1541	4.787	-8.506	10.120	1.00	22.20
ATOM	636	CG	HIS	1541	5.849	-9.555	10.125	1.00	21.32
ATOM	637	CD2	HIS	1541	5.886	-10.789	9.555	1.00	23.29
ATOM	638	ND1	HIS	1541	7.052	-9.413	10.791	1.00	19.41
ATOM	640	CE1	HIS	1541	7.775	-10.509	10.633	1.00	23.61
ATOM	641	NE2	HIS	1541	7.097	-11.355	9.889	1.00	21.81
ATOM	643	C	HIS	1541	4.245	-8.640	12.565	1.00	28.64
ATOM	644	O	HIS	1541	4.290	-7.549	13.132	1.00	30.64
ATOM	645	N	LYS	1542	4.650	-9.791	13.108	1.00	29.47
ATOM	647	CA	LYS	1542	5.200	-9.893	14.457	1.00	28.78
ATOM	648	CB	LYS	1542	5.683	-11.326	14.714	1.00	30.16
ATOM	649	CG	LYS	1542	6.232	-11.572	16.112	1.00	32.63
ATOM	650	CD	LYS	1542	5.277	-11.046	17.155	1.00	42.90
ATOM	651	CE	LYS	1542	5.659	-11.475	18.551	1.00	48.13

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ATOM	652	NZ	LYS	1542	4.726	-10.930	19.564	1.00	54.87
ATOM	656	C	LYS	1542	6.351	-8.928	14.705	1.00	26.54
ATOM	657	O	LYS	1542	6.440	-8.321	15.773	1.00	26.19
ATOM	658	N	ASN	1543	7.193	-8.733	13.697	1.00	24.36
ATOM	660	CA	ASN	1543	8.357	-7.874	13.852	1.00	24.08
ATOM	661	CB	ASN	1543	9.601	-8.596	13.359	1.00	22.69
ATOM	662	CG	ASN	1543	9.781	-9.950	14.029	1.00	22.81
ATOM	663	OD1	ASN	1543	9.664	-10.996	13.388	1.00	23.62
ATOM	664	ND2	ASN	1543	10.028	-9.938	15.324	1.00	24.94
ATOM	667	C	ASN	1543	8.318	-6.429	13.377	1.00	23.48
ATOM	668	O	ASN	1543	9.351	-5.861	13.059	1.00	22.94
ATOM	669	N	ILE	1544	7.130	-5.821	13.380	1.00	24.15
ATOM	671	CA	ILE	1544	6.976	-4.407	13.012	1.00	24.60
ATOM	672	CB	ILE	1544	6.516	-4.191	11.531	1.00	24.90
ATOM	673	CG2	ILE	1544	7.495	-4.852	10.571	1.00	21.57
ATOM	674	CG1	ILE	1544	5.081	-4.688	11.316	1.00	26.66
ATOM	675	CD1	ILE	1544	4.481	-4.321	9.945	1.00	23.98
ATOM	676	C	ILE	1544	5.954	-3.785	13.955	1.00	24.78
ATOM	677	O	ILE	1544	5.160	-4.503	14.558	1.00	27.87
ATOM	678	N	ILE	1545	6.035	-2.474	14.159	1.00	26.39
ATOM	680	CA	ILE	1545	5.089	-1.779	15.025	1.00	26.79
ATOM	681	CB	ILE	1545	5.588	-0.345	15.384	1.00	28.85
ATOM	682	CG2	ILE	1545	4.512	0.449	16.103	1.00	23.60
ATOM	683	CG1	ILE	1545	6.833	-0.423	16.269	1.00	27.20
ATOM	684	CD1	ILE	1545	6.565	-0.990	17.639	1.00	27.12
ATOM	685	C	ILE	1545	3.792	-1.708	14.224	1.00	26.99
ATOM	686	O	ILE	1545	3.720	-1.023	13.197	1.00	27.61
ATOM	687	N	ASN	1546	2.809	-2.495	14.654	1.00	26.70
ATOM	689	CA	ASN	1546	1.514	-2.565	13.983	1.00	26.53
ATOM	690	CB	ASN	1546	0.871	-3.953	14.169	1.00	26.23
ATOM	691	CG	ASN	1546	1.695	-5.072	13.551	1.00	24.96
ATOM	692	OD1	ASN	1546	1.773	-5.206	12.330	1.00	28.08
ATOM	693	ND2	ASN	1546	2.319	-5.872	14.387	1.00	22.38
ATOM	696	C	ASN	1546	0.521	-1.497	14.418	1.00	26.89
ATOM	697	O	ASN	1546	0.610	-0.952	15.523	1.00	27.40
ATOM	698	N	LEU	1547	-0.349	-1.138	13.481	1.00	27.77
ATOM	700	CA	LEU	1547	-1.416	-0.175	13.701	1.00	28.28
ATOM	701	CB	LEU	1547	-1.958	0.313	12.361	1.00	27.04
ATOM	702	CG	LEU	1547	-3.199	1.194	12.408	1.00	25.74
ATOM	703	CD1	LEU	1547	-2.836	2.575	12.950	1.00	27.66
ATOM	704	CD2	LEU	1547	-3.799	1.289	11.014	1.00	23.38
ATOM	705	C	LEU	1547	-2.498	-0.972	14.435	1.00	29.80
ATOM	706	O	LEU	1547	-2.766	-2.135	14.105	1.00	28.63
ATOM	707	N	LEU	1548	-3.088	-0.351	15.448	1.00	29.91
ATOM	709	CA	LEU	1548	-4.114	-0.997	16.256	1.00	28.46
ATOM	710	CB	LEU	1548	-3.735	-0.956	17.749	1.00	26.76
ATOM	711	CG	LEU	1548	-2.460	-1.701	18.162	1.00	22.44
ATOM	712	CD1	LEU	1548	-2.277	-1.554	19.653	1.00	21.91
ATOM	713	CD2	LEU	1548	-2.551	-3.179	17.778	1.00	20.79
ATOM	714	C	LEU	1548	-5.480	-0.365	16.058	1.00	27.31
ATOM	715	O	LEU	1548	-6.489	-1.043	16.193	1.00	28.25
ATOM	716	N	GLY	1549	-5.506	0.925	15.732	1.00	24.02
ATOM	718	CA	GLY	1549	-6.774	1.598	15.553	1.00	24.57
ATOM	719	C	GLY	1549	-6.548	3.077	15.395	1.00	25.19

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ATOM	720	O	GLY	1549	-5.400	3.488	15.231	1.00	28.77
ATOM	721	N	ALA	1550	-7.617	3.875	15.427	1.00	24.66
ATOM	723	CA	ALA	1550	-7.487	5.319	15.282	1.00	24.17
ATOM	724	CB	ALA	1550	-7.206	5.680	13.824	1.00	24.29
ATOM	725	C	ALA	1550	-8.695	6.103	15.765	1.00	23.95
ATOM	726	O	ALA	1550	-9.810	5.590	15.780	1.00	24.95
ATOM	727	N	CYS	1551	-8.444	7.336	16.199	1.00	25.03
ATOM	729	CA	CYS	1551	-9.482	8.270	16.639	1.00	28.21
ATOM	730	CB	CYS	1551	-9.221	8.774	18.055	1.00	26.76
ATOM	731	SG	CYS	1551	-9.378	7.521	19.317	1.00	34.39
ATOM	732	C	CYS	1551	-9.359	9.426	15.656	1.00	29.98
ATOM	733	O	CYS	1551	-8.482	10.281	15.800	1.00	32.14
ATOM	734	N	THR	1552	-10.198	9.412	14.625	1.00	31.09
ATOM	736	CA	THR	1552	-10.135	10.435	13.595	1.00	32.91
ATOM	737	CB	THR	1552	-10.052	9.781	12.189	1.00	32.60
ATOM	738	OG1	THR	1552	-11.276	9.097	11.890	1.00	32.12
ATOM	740	CG2	THR	1552	-8.928	8.768	12.144	1.00	32.74
ATOM	741	C	THR	1552	-11.282	11.419	13.591	1.00	35.26
ATOM	742	O	THR	1552	-11.171	12.525	13.057	1.00	35.10
ATOM	743	N	GLN	1553	-12.397	11.014	14.179	1.00	39.01
ATOM	745	CA	GLN	1553	-13.585	11.846	14.180	1.00	41.97
ATOM	746	CB	GLN	1553	-14.832	10.968	14.020	1.00	41.17
ATOM	747	CG	GLN	1553	-14.915	10.238	12.672	1.00	39.06
ATOM	748	CD	GLN	1553	-14.900	11.200	11.496	1.00	41.84
ATOM	749	OE1	GLN	1553	-15.785	12.045	11.359	1.00	41.92
ATOM	750	NE2	GLN	1553	-13.876	11.090	10.652	1.00	42.33
ATOM	753	C	GLN	1553	-13.727	12.777	15.372	1.00	45.35
ATOM	754	O	GLN	1553	-13.358	12.423	16.489	1.00	47.02
ATOM	755	N	ASP	1554	-14.225	13.981	15.090	1.00	48.60
ATOM	757	CA	ASP	1554	-14.479	15.016	16.084	1.00	50.64
ATOM	758	CB	ASP	1554	-15.832	14.766	16.758	1.00	54.52
ATOM	759	CG	ASP	1554	-17.003	14.955	15.809	1.00	60.54
ATOM	760	OD1	ASP	1554	-18.072	15.409	16.274	1.00	66.04
ATOM	761	OD2	ASP	1554	-16.860	14.661	14.601	1.00	65.09
ATOM	762	C	ASP	1554	-13.395	15.173	17.133	1.00	49.89
ATOM	763	O	ASP	1554	-13.611	14.879	18.310	1.00	51.48
ATOM	764	N	GLY	1555	-12.232	15.643	16.699	1.00	48.40
ATOM	766	CA	GLY	1555	-11.131	15.834	17.617	1.00	46.16
ATOM	767	C	GLY	1555	-9.798	15.626	16.935	1.00	44.64
ATOM	768	O	GLY	1555	-9.737	15.581	15.716	1.00	45.22
ATOM	769	N	PRO	1556	-8.708	15.525	17.702	1.00	44.68
ATOM	770	CD	PRO	1556	-8.672	15.683	19.164	1.00	45.39
ATOM	771	CA	PRO	1556	-7.359	15.326	17.177	1.00	42.95
ATOM	772	CB	PRO	1556	-6.484	15.549	18.411	1.00	43.74
ATOM	773	CG	PRO	1556	-7.354	16.347	19.345	1.00	47.32
ATOM	774	C	PRO	1556	-7.164	13.912	16.665	1.00	42.34
ATOM	775	O	PRO	1556	-7.636	12.953	17.287	1.00	42.75
ATOM	776	N	LEU	1557	-6.451	13.788	15.547	1.00	39.83
ATOM	778	CA	LEU	1557	-6.169	12.490	14.954	1.00	36.64
ATOM	779	CB	LEU	1557	-5.496	12.669	13.587	1.00	34.49
ATOM	780	CG	LEU	1557	-5.009	11.404	12.870	1.00	31.29
ATOM	781	CD1	LEU	1557	-6.169	10.436	12.628	1.00	27.86
ATOM	782	CD2	LEU	1557	-4.314	11.775	11.570	1.00	25.40
ATOM	783	C	LEU	1557	-5.244	11.732	15.894	1.00	35.44

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ATOM	784	O	LEU	1557	-4.210	12.264	16.316	1.00	36.12
ATOM	785	N	TYR	1558	-5.664	10.539	16.292	1.00	32.49
ATOM	787	CA	TYR	1558	-4.861	9.697	17.157	1.00	31.87
ATOM	788	CB	TYR	1558	-5.590	9.348	18.470	1.00	33.93
ATOM	789	CG	TYR	1558	-5.695	10.476	19.471	1.00	35.34
ATOM	790	CD1	TYR	1558	-6.566	10.394	20.565	1.00	37.12
ATOM	791	CE1	TYR	1558	-6.683	11.456	21.479	1.00	36.44
ATOM	792	CD2	TYR	1558	-4.945	11.636	19.317	1.00	37.27
ATOM	793	CE2	TYR	1558	-5.054	12.690	20.213	1.00	39.62
ATOM	794	CZ	TYR	1558	-5.921	12.598	21.289	1.00	40.05
ATOM	795	OH	TYR	1558	-6.008	13.668	22.155	1.00	44.98
ATOM	797	C	TYR	1558	-4.600	8.419	16.387	1.00	31.58
ATOM	798	O	TYR	1558	-5.532	7.750	15.936	1.00	30.22
ATOM	799	N	VAL	1559	-3.331	8.129	16.153	1.00	33.43
ATOM	801	CA	VAL	1559	-2.947	6.907	15.463	1.00	31.42
ATOM	802	CB	VAL	1559	-1.849	7.160	14.419	1.00	32.31
ATOM	803	CG1	VAL	1559	-1.516	5.851	13.675	1.00	26.79
ATOM	804	CG2	VAL	1559	-2.308	8.265	13.453	1.00	30.63
ATOM	805	C	VAL	1559	-2.438	5.979	16.556	1.00	28.67
ATOM	806	O	VAL	1559	-1.393	6.223	17.155	1.00	30.08
ATOM	807	N	ILE	1560	-3.230	4.960	16.852	1.00	25.80
ATOM	809	CA	ILE	1560	-2.915	3.998	17.894	1.00	25.33
ATOM	810	CB	ILE	1560	-4.219	3.443	18.506	1.00	22.34
ATOM	811	CG2	ILE	1560	-3.931	2.695	19.784	1.00	20.36
ATOM	812	CG1	ILE	1560	-5.172	4.603	18.809	1.00	21.34
ATOM	813	CD1	ILE	1560	-6.583	4.190	19.093	1.00	20.68
ATOM	814	C	ILE	1560	-2.073	2.857	17.341	1.00	27.16
ATOM	815	O	ILE	1560	-2.520	2.116	16.455	1.00	29.67
ATOM	816	N	VAL	1561	-0.858	2.714	17.860	1.00	27.69
ATOM	818	CA	VAL	1561	0.060	1.667	17.411	1.00	28.27
ATOM	819	CB	VAL	1561	1.311	2.269	16.696	1.00	27.34
ATOM	820	CG1	VAL	1561	0.892	3.019	15.445	1.00	21.76
ATOM	821	CG2	VAL	1561	2.074	3.201	17.639	1.00	26.00
ATOM	822	C	VAL	1561	0.509	0.809	18.588	1.00	28.70
ATOM	823	O	VAL	1561	0.221	1.139	19.746	1.00	30.52
ATOM	824	N	GLU	1562	1.166	-0.311	18.286	1.00	28.64
ATOM	826	CA	GLU	1562	1.658	-1.220	19.318	1.00	27.77
ATOM	827	CB	GLU	1562	2.278	-2.465	18.693	1.00	24.57
ATOM	828	CG	GLU	1562	1.251	-3.452	18.208	1.00	24.76
ATOM	829	CD	GLU	1562	1.864	-4.641	17.501	1.00	27.27
ATOM	830	OE1	GLU	1562	1.272	-5.739	17.580	1.00	28.27
ATOM	831	OE2	GLU	1562	2.920	-4.487	16.849	1.00	29.25
ATOM	832	C	GLU	1562	2.674	-0.538	20.217	1.00	28.79
ATOM	833	O	GLU	1562	3.453	0.292	19.760	1.00	29.38
ATOM	834	N	TYR	1563	2.627	-0.871	21.503	1.00	30.84
ATOM	836	CA	TYR	1563	3.534	-0.304	22.493	1.00	31.43
ATOM	837	CB	TYR	1563	2.782	-0.088	23.799	1.00	32.10
ATOM	838	CG	TYR	1563	3.632	0.376	24.952	1.00	33.93
ATOM	839	CD1	TYR	1563	4.366	1.552	24.873	1.00	34.85
ATOM	840	CE1	TYR	1563	5.140	1.992	25.947	1.00	37.53
ATOM	841	CD2	TYR	1563	3.683	-0.356	26.136	1.00	34.81
ATOM	842	CE2	TYR	1563	4.452	0.072	27.211	1.00	34.01
ATOM	843	CZ	TYR	1563	5.173	1.245	27.113	1.00	35.79
ATOM	844	OH	TYR	1563	5.920	1.677	28.184	1.00	39.10

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ATOM	846	C	TYR	1563	4.767	-1.166	22.731	1.00	31.38
ATOM	847	O	TYR	1563	4.672	-2.385	22.905	1.00	30.73
ATOM	848	N	ALA	1564	5.930	-0.525	22.725	1.00	32.23
ATOM	850	CA	ALA	1564	7.198	-1.212	22.953	1.00	35.90
ATOM	851	CB	ALA	1564	8.178	-0.866	21.833	1.00	36.44
ATOM	852	C	ALA	1564	7.711	-0.719	24.307	1.00	36.52
ATOM	853	O	ALA	1564	8.332	0.349	24.403	1.00	39.16
ATOM	854	N	SER	1565	7.424	-1.482	25.359	1.00	34.62
ATOM	856	CA	SER	1565	7.801	-1.071	26.700	1.00	34.91
ATOM	857	CB	SER	1565	7.124	-1.945	27.750	1.00	32.11
ATOM	858	OG	SER	1565	7.606	-3.271	27.696	1.00	32.92
ATOM	860	C	SER	1565	9.288	-0.968	26.996	1.00	35.56
ATOM	861	O	SER	1565	9.674	-0.219	27.886	1.00	38.69
ATOM	862	N	LYS	1566	10.127	-1.673	26.243	1.00	33.70
ATOM	864	CA	LYS	1566	11.557	-1.625	26.526	1.00	31.40
ATOM	865	CB	LYS	1566	12.137	-3.033	26.530	1.00	30.56
ATOM	866	CG	LYS	1566	11.555	-3.869	27.664	1.00	32.32
ATOM	867	CD	LYS	1566	11.997	-5.308	27.599	1.00	36.47
ATOM	868	CE	LYS	1566	11.632	-6.031	28.872	1.00	36.97
ATOM	869	NZ	LYS	1566	12.104	-7.436	28.804	1.00	41.62
ATOM	873	C	LYS	1566	12.380	-0.664	25.683	1.00	32.18
ATOM	874	O	LYS	1566	13.616	-0.691	25.715	1.00	32.57
ATOM	875	N	GLY	1567	11.686	0.223	24.973	1.00	33.39
ATOM	877	CA	GLY	1567	12.345	1.224	24.156	1.00	32.13
ATOM	878	C	GLY	1567	13.074	0.719	22.928	1.00	31.70
ATOM	879	O	GLY	1567	12.912	-0.430	22.530	1.00	33.30
ATOM	880	N	ASN	1568	13.883	1.589	22.331	1.00	31.08
ATOM	882	CA	ASN	1568	14.632	1.230	21.139	1.00	31.00
ATOM	883	CB	ASN	1568	15.066	2.478	20.365	1.00	31.30
ATOM	884	CG	ASN	1568	16.127	3.271	21.074	1.00	30.47
ATOM	885	OD1	ASN	1568	17.130	2.733	21.508	1.00	32.19
ATOM	886	ND2	ASN	1568	15.934	4.580	21.144	1.00	32.13
ATOM	889	C	ASN	1568	15.802	0.295	21.393	1.00	30.62
ATOM	890	O	ASN	1568	16.357	0.256	22.483	1.00	32.91
ATOM	891	N	LEU	1569	16.193	-0.428	20.354	1.00	30.92
ATOM	893	CA	LEU	1569	17.269	-1.403	20.417	1.00	31.22
ATOM	894	CB	LEU	1569	17.418	-2.083	19.054	1.00	29.57
ATOM	895	CG	LEU	1569	18.415	-3.231	18.893	1.00	29.22
ATOM	896	CD1	LEU	1569	18.284	-4.261	20.024	1.00	21.30
ATOM	897	CD2	LEU	1569	18.184	-3.863	17.523	1.00	24.99
ATOM	898	C	LEU	1569	18.609	-0.838	20.878	1.00	32.44
ATOM	899	O	LEU	1569	19.328	-1.499	21.618	1.00	33.12
ATOM	900	N	ARG	1570	18.954	0.370	20.432	1.00	33.24
ATOM	902	CA	ARG	1570	20.218	0.983	20.834	1.00	33.01
ATOM	903	CB	ARG	1570	20.348	2.394	20.256	1.00	32.36
ATOM	904	CG	ARG	1570	21.586	3.129	20.758	1.00	38.28
ATOM	905	CD	ARG	1570	21.672	4.538	20.221	1.00	41.93
ATOM	906	NE	ARG	1570	20.428	5.278	20.412	1.00	49.82
ATOM	908	CZ	ARG	1570	19.975	5.721	21.584	1.00	52.37
ATOM	909	NH1	ARG	1570	20.659	5.510	22.712	1.00	51.61
ATOM	912	NH2	ARG	1570	18.824	6.377	21.622	1.00	53.28
ATOM	915	C	ARG	1570	20.308	1.023	22.371	1.00	33.90
ATOM	916	O	ARG	1570	21.184	0.391	22.970	1.00	33.17
ATOM	917	N	GLU	1571	19.359	1.730	22.981	1.00	33.45

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ATOM	919	CA	GLU	1571	19.284	1.861	24.432	1.00	34.87
ATOM	920	CB	GLU	1571	18.052	2.688	24.794	1.00	35.83
ATOM	921	CG	GLU	1571	18.158	4.145	24.354	1.00	41.61
ATOM	922	CD	GLU	1571	16.814	4.870	24.318	1.00	47.33
ATOM	923	OE1	GLU	1571	15.759	4.199	24.362	1.00	50.68
ATOM	924	OE2	GLU	1571	16.812	6.120	24.218	1.00	48.07
ATOM	925	C	GLU	1571	19.223	0.487	25.098	1.00	34.39
ATOM	926	O	GLU	1571	19.968	0.202	26.041	1.00	34.04
ATOM	927	N	TYR	1572	18.363	-0.376	24.572	1.00	33.49
ATOM	929	CA	TYR	1572	18.204	-1.728	25.083	1.00	30.45
ATOM	930	CB	TYR	1572	17.210	-2.495	24.202	1.00	28.13
ATOM	931	CG	TYR	1572	17.074	-3.971	24.487	1.00	25.80
ATOM	932	CD1	TYR	1572	16.105	-4.443	25.371	1.00	28.92
ATOM	933	CE1	TYR	1572	15.954	-5.804	25.618	1.00	30.03
ATOM	934	CD2	TYR	1572	17.899	-4.899	23.863	1.00	24.61
ATOM	935	CE2	TYR	1572	17.760	-6.260	24.102	1.00	26.05
ATOM	936	CZ	TYR	1572	16.790	-6.705	24.982	1.00	29.23
ATOM	937	OH	TYR	1572	16.651	-8.052	25.227	1.00	33.74
ATOM	939	C	TYR	1572	19.549	-2.447	25.113	1.00	31.30
ATOM	940	O	TYR	1572	19.880	-3.126	26.090	1.00	32.43
ATOM	941	N	LEU	1573	20.334	-2.266	24.058	1.00	29.68
ATOM	943	CA	LEU	1573	21.625	-2.923	23.972	1.00	30.04
ATOM	944	CB	LEU	1573	22.145	-2.909	22.529	1.00	26.13
ATOM	945	CG	LEU	1573	21.532	-3.870	21.490	1.00	25.24
ATOM	946	CD1	LEU	1573	22.097	-3.563	20.113	1.00	19.70
ATOM	947	CD2	LEU	1573	21.807	-5.317	21.839	1.00	22.05
ATOM	948	C	LEU	1573	22.645	-2.308	24.927	1.00	34.47
ATOM	949	O	LEU	1573	23.354	-3.031	25.644	1.00	34.95
ATOM	950	N	GLN	1574	22.691	-0.980	24.978	1.00	35.47
ATOM	952	CA	GLN	1574	23.639	-0.293	25.850	1.00	37.09
ATOM	953	CB	GLN	1574	23.601	1.206	25.579	1.00	36.70
ATOM	954	CG	GLN	1574	24.033	1.559	24.171	1.00	39.77
ATOM	955	CD	GLN	1574	23.960	3.045	23.884	1.00	41.51
ATOM	956	OE1	GLN	1574	23.592	3.837	24.751	1.00	42.57
ATOM	957	NE2	GLN	1574	24.288	3.431	22.652	1.00	41.34
ATOM	960	C	GLN	1574	23.400	-0.588	27.332	1.00	37.85
ATOM	961	O	GLN	1574	24.343	-0.801	28.090	1.00	38.87
ATOM	962	N	ALA	1575	22.131	-0.667	27.720	1.00	39.01
ATOM	964	CA	ALA	1575	21.740	-0.944	29.098	1.00	37.00
ATOM	965	CB	ALA	1575	20.261	-0.678	29.273	1.00	35.71
ATOM	966	C	ALA	1575	22.061	-2.359	29.559	1.00	39.14
ATOM	967	O	ALA	1575	21.839	-2.692	30.719	1.00	43.81
ATOM	968	N	ARG	1576	22.563	-3.201	28.665	1.00	38.39
ATOM	970	CA	ARG	1576	22.897	-4.568	29.032	1.00	37.71
ATOM	971	CB	ARG	1576	21.994	-5.544	28.290	1.00	38.26
ATOM	972	CG	ARG	1576	20.555	-5.383	28.700	1.00	38.00
ATOM	973	CD	ARG	1576	19.653	-6.282	27.920	1.00	34.74
ATOM	974	NE	ARG	1576	18.279	-6.190	28.388	1.00	32.88
ATOM	976	CZ	ARG	1576	17.572	-5.066	28.442	1.00	34.02
ATOM	977	NH1	ARG	1576	18.114	-3.913	28.068	1.00	35.57
ATOM	980	NH2	ARG	1576	16.298	-5.102	28.800	1.00	36.71
ATOM	983	C	ARG	1576	24.365	-4.927	28.828	1.00	39.59
ATOM	984	O	ARG	1576	24.735	-6.113	28.788	1.00	39.83
ATOM	985	N	ARG	1577	25.200	-3.900	28.687	1.00	38.82

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ATOM	987	CA	ARG	1577	26.631	-4.101	28.520	1.00	39.07
ATOM	988	CB	ARG	1577	27.310	-2.797	28.090	1.00	34.91
ATOM	989	CG	ARG	1577	27.033	-2.323	26.681	1.00	33.87
ATOM	990	CD	ARG	1577	27.730	-0.981	26.428	1.00	33.06
ATOM	991	NE	ARG	1577	27.722	-0.612	25.015	1.00	38.87
ATOM	993	CZ	ARG	1577	28.174	0.538	24.517	1.00	39.76
ATOM	994	NH1	ARG	1577	28.683	1.470	25.305	1.00	40.68
ATOM	997	NH2	ARG	1577	28.122	0.758	23.213	1.00	43.26
ATOM	1000	C	ARG	1577	27.181	-4.501	29.885	1.00	41.58
ATOM	1001	O	ARG	1577	26.586	-4.181	30.917	1.00	42.48
ATOM	1002	N	PRO	1578	28.294	-5.249	29.919	1.00	43.07
ATOM	1003	CD	PRO	1578	29.110	-5.812	28.823	1.00	43.36
ATOM	1004	CA	PRO	1578	28.839	-5.626	31.223	1.00	42.69
ATOM	1005	CB	PRO	1578	29.966	-6.595	30.857	1.00	42.22
ATOM	1006	CG	PRO	1578	30.412	-6.103	29.516	1.00	43.64
ATOM	1007	C	PRO	1578	29.366	-4.350	31.882	1.00	43.37
ATOM	1008	O	PRO	1578	29.530	-3.319	31.215	1.00	42.50
ATOM	1009	N	PRO	1579	29.596	-4.380	33.198	1.00	45.24
ATOM	1010	CD	PRO	1579	29.279	-5.435	34.174	1.00	44.69
ATOM	1011	CA	PRO	1579	30.099	-3.187	33.882	1.00	46.27
ATOM	1012	CB	PRO	1579	29.979	-3.567	35.353	1.00	45.78
ATOM	1013	CG	PRO	1579	28.894	-4.615	35.361	1.00	46.15
ATOM	1014	C	PRO	1579	31.548	-2.869	33.500	1.00	48.38
ATOM	1015	O	PRO	1579	32.410	-3.753	33.478	1.00	50.64
ATOM	1016	N	GLU	1592	19.022	-5.398	32.495	1.00	65.98
ATOM	1018	CA	GLU	1592	20.442	-5.048	32.492	1.00	64.80
ATOM	1019	CB	GLU	1592	20.796	-4.241	33.740	1.00	67.30
ATOM	1020	C	GLU	1592	21.351	-6.275	32.371	1.00	63.80
ATOM	1021	O	GLU	1592	22.545	-6.149	32.089	1.00	65.21
ATOM	1022	N	GLU	1593	20.789	-7.458	32.607	1.00	61.44
ATOM	1024	CA	GLU	1593	21.560	-8.691	32.495	1.00	60.82
ATOM	1025	CB	GLU	1593	20.681	-9.899	32.807	1.00	61.47
ATOM	1026	C	GLU	1593	22.144	-8.803	31.089	1.00	59.12
ATOM	1027	O	GLU	1593	21.468	-8.525	30.097	1.00	59.49
ATOM	1028	N	GLN	1594	23.408	-9.201	31.017	1.00	57.33
ATOM	1030	CA	GLN	1594	24.103	-9.334	29.744	1.00	55.30
ATOM	1031	CB	GLN	1594	25.523	-9.880	29.957	1.00	54.87
ATOM	1032	CG	GLN	1594	26.438	-8.959	30.757	1.00	53.34
ATOM	1033	CD	GLN	1594	27.704	-9.660	31.248	1.00	55.27
ATOM	1034	OE1	GLN	1594	28.256	-10.536	30.572	1.00	56.47
ATOM	1035	NE2	GLN	1594	28.166	-9.275	32.434	1.00	51.46
ATOM	1038	C	GLN	1594	23.336	-10.229	28.781	1.00	52.29
ATOM	1039	O	GLN	1594	22.648	-11.166	29.190	1.00	52.56
ATOM	1040	N	LEU	1595	23.447	-9.913	27.499	1.00	49.40
ATOM	1042	CA	LEU	1595	22.783	-10.676	26.455	1.00	46.00
ATOM	1043	CB	LEU	1595	22.452	-9.760	25.274	1.00	42.94
ATOM	1044	CG	LEU	1595	21.390	-8.711	25.626	1.00	43.90
ATOM	1045	CD1	LEU	1595	21.495	-7.484	24.743	1.00	39.46
ATOM	1046	CD2	LEU	1595	20.005	-9.347	25.569	1.00	41.86
ATOM	1047	C	LEU	1595	23.741	-11.762	26.029	1.00	43.96
ATOM	1048	O	LEU	1595	24.950	-11.550	26.043	1.00	44.24
ATOM	1049	N	SER	1596	23.217	-12.941	25.714	1.00	43.29
ATOM	1051	CA	SER	1596	24.076	-14.027	25.275	1.00	42.40
ATOM	1052	CB	SER	1596	23.388	-15.374	25.484	1.00	41.83

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ATOM	1053	OG	SER	1596	22.218	-15.483	24.697	1.00	44.25
ATOM	1055	C	SER	1596	24.392	-13.817	23.800	1.00	42.64
ATOM	1056	O	SER	1596	23.857	-12.900	23.171	1.00	43.14
ATOM	1057	N	SER	1597	25.277	-14.645	23.255	1.00	42.59
ATOM	1059	CA	SER	1597	25.629	-14.553	21.850	1.00	42.91
ATOM	1060	CB	SER	1597	26.739	-15.547	21.516	1.00	45.26
ATOM	1061	OG	SER	1597	27.812	-15.436	22.431	1.00	56.41
ATOM	1063	C	SER	1597	24.380	-14.909	21.048	1.00	42.35
ATOM	1064	O	SER	1597	24.113	-14.322	20.003	1.00	43.71
ATOM	1065	N	LYS	1598	23.621	-15.881	21.544	1.00	40.61
ATOM	1067	CA	LYS	1598	22.405	-16.298	20.867	1.00	38.61
ATOM	1068	CB	LYS	1598	21.848	-17.575	21.483	1.00	36.33
ATOM	1069	CG	LYS	1598	21.135	-18.439	20.468	1.00	40.09
ATOM	1070	CD	LYS	1598	20.213	-19.434	21.118	1.00	43.39
ATOM	1071	CE	LYS	1598	19.766	-20.494	20.122	1.00	48.25
ATOM	1072	NZ	LYS	1598	20.930	-21.290	19.623	1.00	50.46
ATOM	1076	C	LYS	1598	21.348	-15.194	20.895	1.00	38.17
ATOM	1077	O	LYS	1598	20.579	-15.053	19.945	1.00	41.27
ATOM	1078	N	ASP	1599	21.321	-14.408	21.969	1.00	35.90
ATOM	1080	CA	ASP	1599	20.366	-13.307	22.099	1.00	34.08
ATOM	1081	CB	ASP	1599	20.450	-12.661	23.477	1.00	37.83
ATOM	1082	CG	ASP	1599	19.822	-13.505	24.562	1.00	39.93
ATOM	1083	OD1	ASP	1599	20.089	-13.217	25.742	1.00	45.85
ATOM	1084	OD2	ASP	1599	19.060	-14.444	24.240	1.00	41.06
ATOM	1085	C	ASP	1599	20.634	-12.243	21.061	1.00	32.37
ATOM	1086	O	ASP	1599	19.704	-11.701	20.466	1.00	32.58
ATOM	1087	N	LEU	1600	21.915	-11.945	20.873	1.00	30.45
ATOM	1089	CA	LEU	1600	22.355	-10.948	19.902	1.00	29.59
ATOM	1090	CB	LEU	1600	23.841	-10.654	20.097	1.00	28.59
ATOM	1091	CG	LEU	1600	24.238	-10.057	21.449	1.00	24.59
ATOM	1092	CD1	LEU	1600	25.747	-9.869	21.522	1.00	18.40
ATOM	1093	CD2	LEU	1600	23.529	-8.745	21.626	1.00	21.71
ATOM	1094	C	LEU	1600	22.073	-11.393	18.458	1.00	28.54
ATOM	1095	O	LEU	1600	21.578	-10.613	17.648	1.00	25.59
ATOM	1096	N	VAL	1601	22.377	-12.645	18.134	1.00	29.13
ATOM	1098	CA	VAL	1601	22.111	-13.154	16.793	1.00	29.74
ATOM	1099	CB	VAL	1601	22.780	-14.513	16.551	1.00	29.63
ATOM	1100	CG1	VAL	1601	22.615	-14.922	15.105	1.00	29.30
ATOM	1101	CG2	VAL	1601	24.259	-14.422	16.873	1.00	28.52
ATOM	1102	C	VAL	1601	20.591	-13.247	16.564	1.00	29.98
ATOM	1103	O	VAL	1601	20.106	-13.040	15.452	1.00	29.73
ATOM	1104	N	SER	1602	19.855	-13.493	17.645	1.00	30.97
ATOM	1106	CA	SER	1602	18.399	-13.576	17.607	1.00	29.64
ATOM	1107	CB	SER	1602	17.894	-14.141	18.925	1.00	30.45
ATOM	1108	OG	SER	1602	16.483	-14.158	18.962	1.00	39.63
ATOM	1110	C	SER	1602	17.784	-12.192	17.343	1.00	29.30
ATOM	1111	O	SER	1602	16.772	-12.071	16.641	1.00	28.74
ATOM	1112	N	CYS	1603	18.385	-11.157	17.925	1.00	27.68
ATOM	1114	CA	CYS	1603	17.931	-9.783	17.717	1.00	27.32
ATOM	1115	CB	CYS	1603	18.791	-8.790	18.516	1.00	25.40
ATOM	1116	SG	CYS	1603	18.472	-7.039	18.177	0.50	20.76
ATOM	1117	C	CYS	1603	18.057	-9.468	16.225	1.00	28.34
ATOM	1118	O	CYS	1603	17.134	-8.926	15.629	1.00	29.70
ATOM	1119	N	ALA	1604	19.192	-9.837	15.627	1.00	29.36

PRT1

ATOM	1121	CA	ALA	1604	19.438	-9.601	14.195	1.00	28.78
ATOM	1122	CB	ALA	1604	20.861	-10.066	13.808	1.00	22.61
ATOM	1123	C	ALA	1604	18.386	-10.304	13.324	1.00	30.14
ATOM	1124	O	ALA	1604	17.792	-9.690	12.426	1.00	31.64
ATOM	1125	N	TYR	1605	18.156	-11.587	13.605	1.00	29.84
ATOM	1127	CA	TYR	1605	17.179	-12.392	12.874	1.00	28.26
ATOM	1128	CB	TYR	1605	17.107	-13.789	13.488	1.00	28.74
ATOM	1129	CG	TYR	1605	16.018	-14.673	12.912	1.00	31.12
ATOM	1130	CD1	TYR	1605	16.152	-15.256	11.650	1.00	32.53
ATOM	1131	CE1	TYR	1605	15.144	-16.067	11.121	1.00	30.84
ATOM	1132	CD2	TYR	1605	14.853	-14.926	13.634	1.00	31.21
ATOM	1133	CE2	TYR	1605	13.850	-15.734	13.116	1.00	29.69
ATOM	1134	CZ	TYR	1605	14.002	-16.296	11.864	1.00	30.82
ATOM	1135	OH	TYR	1605	12.990	-17.069	11.359	1.00	33.77
ATOM	1137	C	TYR	1605	15.788	-11.758	12.853	1.00	27.33
ATOM	1138	O	TYR	1605	15.152	-11.691	11.805	1.00	27.94
ATOM	1139	N	GLN	1606	15.323	-11.292	14.007	1.00	27.93
ATOM	1141	CA	GLN	1606	14.008	-10.659	14.115	1.00	27.20
ATOM	1142	CB	GLN	1606	13.686	-10.335	15.570	1.00	26.40
ATOM	1143	CG	GLN	1606	13.301	-11.556	16.402	1.00	28.12
ATOM	1144	CD	GLN	1606	13.114	-11.215	17.865	1.00	30.41
ATOM	1145	OE1	GLN	1606	12.188	-10.489	18.234	1.00	34.34
ATOM	1146	NE2	GLN	1606	14.008	-11.701	18.700	1.00	31.44
ATOM	1149	C	GLN	1606	13.906	-9.397	13.275	1.00	29.67
ATOM	1150	O	GLN	1606	12.884	-9.148	12.622	1.00	30.74
ATOM	1151	N	VAL	1607	14.970	-8.602	13.281	1.00	29.59
ATOM	1153	CA	VAL	1607	14.996	-7.377	12.501	1.00	27.00
ATOM	1154	CB	VAL	1607	16.235	-6.544	12.842	1.00	27.20
ATOM	1155	CG1	VAL	1607	16.382	-5.397	11.859	1.00	28.11
ATOM	1156	CG2	VAL	1607	16.113	-5.996	14.266	1.00	24.79
ATOM	1157	C	VAL	1607	14.966	-7.725	11.014	1.00	28.02
ATOM	1158	O	VAL	1607	14.229	-7.108	10.241	1.00	28.28
ATOM	1159	N	ALA	1608	15.736	-8.741	10.626	1.00	27.56
ATOM	1161	CA	ALA	1608	15.787	-9.206	9.236	1.00	27.36
ATOM	1162	CB	ALA	1608	16.801	-10.339	9.095	1.00	26.25
ATOM	1163	C	ALA	1608	14.402	-9.674	8.779	1.00	28.58
ATOM	1164	O	ALA	1608	14.013	-9.446	7.624	1.00	29.11
ATOM	1165	N	ARG	1609	13.660	-10.326	9.680	1.00	28.88
ATOM	1167	CA	ARG	1609	12.306	-10.797	9.376	1.00	27.17
ATOM	1168	CB	ARG	1609	11.797	-11.731	10.464	1.00	29.68
ATOM	1169	CG	ARG	1609	12.458	-13.062	10.439	1.00	31.65
ATOM	1170	CD	ARG	1609	11.612	-14.049	11.177	1.00	38.21
ATOM	1171	NE	ARG	1609	10.856	-14.897	10.269	1.00	41.10
ATOM	1173	CZ	ARG	1609	10.048	-15.872	10.667	1.00	41.97
ATOM	1174	NH1	ARG	1609	9.886	-16.125	11.959	1.00	40.69
ATOM	1177	NH2	ARG	1609	9.411	-16.609	9.770	1.00	43.57
ATOM	1180	C	ARG	1609	11.312	-9.654	9.183	1.00	25.38
ATOM	1181	O	ARG	1609	10.480	-9.693	8.260	1.00	25.75
ATOM	1182	N	GLY	1610	11.365	-8.661	10.070	1.00	24.03
ATOM	1184	CA	GLY	1610	10.480	-7.517	9.939	1.00	21.74
ATOM	1185	C	GLY	1610	10.734	-6.864	8.592	1.00	23.32
ATOM	1186	O	GLY	1610	9.805	-6.540	7.850	1.00	23.39
ATOM	1187	N	MET	1611	12.016	-6.714	8.265	1.00	24.48
ATOM	1189	CA	MET	1611	12.453	-6.125	7.002	1.00	23.13

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ATOM	1190	CB	MET	1611	13.949	-5.860	7.035	1.00	19.46
ATOM	1191	CG	MET	1611	14.339	-4.671	7.910	1.00	22.46
ATOM	1192	SD	MET	1611	13.457	-3.123	7.536	1.00	25.27
ATOM	1193	CE	MET	1611	13.900	-2.801	5.876	1.00	22.25
ATOM	1194	C	MET	1611	12.100	-7.005	5.811	1.00	24.87
ATOM	1195	O	MET	1611	11.699	-6.497	4.755	1.00	24.09
ATOM	1196	N	GLU	1612	12.230	-8.321	5.975	1.00	25.48
ATOM	1198	CA	GLU	1612	11.894	-9.232	4.890	1.00	25.42
ATOM	1199	CB	GLU	1612	12.155	-10.691	5.288	1.00	23.41
ATOM	1200	CG	GLU	1612	11.664	-11.679	4.232	1.00	25.14
ATOM	1201	CD	GLU	1612	11.872	-13.141	4.599	1.00	28.60
ATOM	1202	OE1	GLU	1612	11.637	-13.514	5.777	1.00	30.10
ATOM	1203	OE2	GLU	1612	12.244	-13.928	3.694	1.00	29.53
ATOM	1204	C	GLU	1612	10.418	-9.021	4.521	1.00	26.92
ATOM	1205	O	GLU	1612	10.065	-8.928	3.343	1.00	29.61
ATOM	1206	N	TYR	1613	9.576	-8.884	5.542	1.00	27.88
ATOM	1208	CA	TYR	1613	8.154	-8.675	5.337	1.00	23.82
ATOM	1209	CB	TYR	1613	7.415	-8.769	6.667	1.00	24.17
ATOM	1210	CG	TYR	1613	5.941	-8.492	6.545	1.00	23.73
ATOM	1211	CD1	TYR	1613	5.064	-9.483	6.096	1.00	22.17
ATOM	1212	CE1	TYR	1613	3.698	-9.235	5.965	1.00	21.08
ATOM	1213	CD2	TYR	1613	5.419	-7.237	6.865	1.00	23.16
ATOM	1214	CE2	TYR	1613	4.054	-6.976	6.736	1.00	26.38
ATOM	1215	CZ	TYR	1613	3.200	-7.981	6.287	1.00	23.16
ATOM	1216	OH	TYR	1613	1.855	-7.725	6.149	1.00	25.50
ATOM	1218	C	TYR	1613	7.885	-7.327	4.670	1.00	23.17
ATOM	1219	O	TYR	1613	7.147	-7.246	3.689	1.00	24.21
ATOM	1220	N	LEU	1614	8.481	-6.266	5.206	1.00	23.04
ATOM	1222	CA	LEU	1614	8.316	-4.920	4.652	1.00	21.81
ATOM	1223	CB	LEU	1614	9.107	-3.906	5.484	1.00	19.94
ATOM	1224	CG	LEU	1614	8.609	-3.616	6.902	1.00	21.94
ATOM	1225	CD1	LEU	1614	9.580	-2.719	7.654	1.00	14.28
ATOM	1226	CD2	LEU	1614	7.227	-2.977	6.814	1.00	17.45
ATOM	1227	C	LEU	1614	8.764	-4.858	3.182	1.00	23.74
ATOM	1228	O	LEU	1614	8.169	-4.150	2.367	1.00	25.26
ATOM	1229	N	ALA	1615	9.831	-5.587	2.862	1.00	25.00
ATOM	1231	CA	ALA	1615	10.357	-5.644	1.502	1.00	23.04
ATOM	1232	CB	ALA	1615	11.710	-6.360	1.483	1.00	20.02
ATOM	1233	C	ALA	1615	9.351	-6.357	0.605	1.00	23.15
ATOM	1234	O	ALA	1615	9.076	-5.891	-0.503	1.00	25.25
ATOM	1235	N	SER	1616	8.754	-7.441	1.104	1.00	23.64
ATOM	1237	CA	SER	1616	7.758	-8.199	0.337	1.00	23.60
ATOM	1238	CB	SER	1616	7.346	-9.453	1.107	1.00	22.46
ATOM	1239	OG	SER	1616	6.531	-9.131	2.224	1.00	26.66
ATOM	1241	C	SER	1616	6.505	-7.369	0.025	1.00	25.45
ATOM	1242	O	SER	1616	5.813	-7.607	-0.967	1.00	26.67
ATOM	1243	N	LYS	1617	6.193	-6.436	0.916	1.00	25.47
ATOM	1245	CA	LYS	1617	5.051	-5.551	0.781	1.00	25.04
ATOM	1246	CB	LYS	1617	4.513	-5.183	2.163	1.00	26.30
ATOM	1247	CG	LYS	1617	3.778	-6.318	2.851	1.00	28.58
ATOM	1248	CD	LYS	1617	2.438	-6.530	2.169	1.00	33.00
ATOM	1249	CE	LYS	1617	1.652	-7.676	2.764	1.00	38.57
ATOM	1250	NZ	LYS	1617	2.167	-8.987	2.300	1.00	45.15
ATOM	1254	C	LYS	1617	5.417	-4.293	0.002	1.00	26.34

ATOM	1255	O	LYS	1617	4.649	-3.336	-0.034	1.00	26.77
ATOM	1256	N	LYS	1618	6.592	-4.319	-0.632	1.00	27.17
ATOM	1258	CA	LYS	1618	7.084	-3.197	-1.447	1.00	28.20
ATOM	1259	CB	LYS	1618	6.053	-2.819	-2.528	1.00	28.42
ATOM	1260	CG	LYS	1618	5.971	-3.749	-3.730	1.00	26.63
ATOM	1261	CD	LYS	1618	5.573	-5.163	-3.364	1.00	30.45
ATOM	1262	CE	LYS	1618	5.636	-6.087	-4.570	1.00	32.50
ATOM	1263	NZ	LYS	1618	4.621	-5.729	-5.600	1.00	34.89
ATOM	1267	C	LYS	1618	7.466	-1.951	-0.643	1.00	28.78
ATOM	1268	O	LYS	1618	7.556	-0.848	-1.199	1.00	28.78
ATOM	1269	N	CYS	1619	7.753	-2.130	0.646	1.00	29.26
ATOM	1271	CA	CYS	1619	8.111	-1.022	1.522	1.00	28.32
ATOM	1272	CB	CYS	1619	7.391	-1.173	2.873	1.00	26.33
ATOM	1273	SG	CYS	1619	7.754	0.105	4.136	1.00	27.82
ATOM	1274	C	CYS	1619	9.622	-0.841	1.728	1.00	29.15
ATOM	1275	O	CYS	1619	10.336	-1.786	2.072	1.00	29.55
ATOM	1276	N	ILE	1620	10.096	0.378	1.457	1.00	29.39
ATOM	1278	CA	ILE	1620	11.502	0.761	1.625	1.00	27.44
ATOM	1279	CB	ILE	1620	12.030	1.543	0.381	1.00	25.37
ATOM	1280	CG2	ILE	1620	13.521	1.806	0.506	1.00	19.80
ATOM	1281	CG1	ILE	1620	11.767	0.764	-0.913	1.00	25.40
ATOM	1282	CD1	ILE	1620	12.100	1.557	-2.164	1.00	27.51
ATOM	1283	C	ILE	1620	11.553	1.686	2.855	1.00	26.56
ATOM	1284	O	ILE	1620	11.011	2.792	2.833	1.00	26.68
ATOM	1285	N	HIS	1621	12.193	1.210	3.916	1.00	26.31
ATOM	1287	CA	HIS	1621	12.297	1.967	5.162	1.00	25.00
ATOM	1288	CB	HIS	1621	13.081	1.174	6.210	1.00	23.08
ATOM	1289	CG	HIS	1621	12.848	1.633	7.618	1.00	23.21
ATOM	1290	CD2	HIS	1621	12.224	1.027	8.656	1.00	22.69
ATOM	1291	ND1	HIS	1621	13.260	2.862	8.088	1.00	25.34
ATOM	1293	CE1	HIS	1621	12.909	2.993	9.356	1.00	24.18
ATOM	1294	NE2	HIS	1621	12.273	1.891	9.719	1.00	25.86
ATOM	1296	C	HIS	1621	12.963	3.316	4.976	1.00	25.09
ATOM	1297	O	HIS	1621	12.408	4.328	5.349	1.00	28.21
ATOM	1298	N	ARG	1622	14.162	3.315	4.402	1.00	26.09
ATOM	1300	CA	ARG	1622	14.976	4.520	4.183	1.00	26.50
ATOM	1301	CB	ARG	1622	14.180	5.670	3.558	1.00	23.52
ATOM	1302	CG	ARG	1622	13.673	5.326	2.202	1.00	23.81
ATOM	1303	CD	ARG	1622	12.995	6.494	1.551	1.00	28.42
ATOM	1304	NE	ARG	1622	12.677	6.170	0.180	1.00	32.52
ATOM	1306	CZ	ARG	1622	11.623	5.455	-0.197	1.00	32.34
ATOM	1307	NH1	ARG	1622	10.774	4.994	0.711	1.00	30.07
ATOM	1310	NH2	ARG	1622	11.460	5.138	-1.489	1.00	28.30
ATOM	1313	C	ARG	1622	15.740	4.993	5.423	1.00	26.31
ATOM	1314	O	ARG	1622	16.698	5.757	5.313	1.00	26.19
ATOM	1315	N	ASP	1623	15.379	4.495	6.596	1.00	27.41
ATOM	1317	CA	ASP	1623	16.114	4.879	7.788	1.00	29.94
ATOM	1318	CB	ASP	1623	15.562	6.155	8.430	1.00	34.83
ATOM	1319	CG	ASP	1623	16.481	6.689	9.533	1.00	38.84
ATOM	1320	OD1	ASP	1623	15.971	7.265	10.514	1.00	44.51
ATOM	1321	OD2	ASP	1623	17.721	6.514	9.423	1.00	37.59
ATOM	1322	C	ASP	1623	16.203	3.763	8.812	1.00	28.71
ATOM	1323	O	ASP	1623	15.845	3.927	9.990	1.00	26.21
ATOM	1324	N	LEU	1624	16.735	2.633	8.357	1.00	26.82

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ATOM	1326	CA	LEU	1624	16.905	1.469	9.216	1.00	25.91
ATOM	1327	CB	LEU	1624	17.025	0.209	8.367	1.00	23.35
ATOM	1328	CG	LEU	1624	17.089	-1.107	9.127	1.00	21.09
ATOM	1329	CD1	LEU	1624	15.824	-1.303	10.009	1.00	14.44
ATOM	1330	CD2	LEU	1624	17.282	-2.215	8.101	1.00	18.30
ATOM	1331	C	LEU	1624	18.136	1.640	10.105	1.00	24.93
ATOM	1332	O	LEU	1624	19.235	1.897	9.611	1.00	25.58
ATOM	1333	N	ALA	1625	17.912	1.557	11.416	1.00	26.30
ATOM	1335	CA	ALA	1625	18.945	1.702	12.445	1.00	23.59
ATOM	1336	CB	ALA	1625	19.271	3.174	12.654	1.00	15.82
ATOM	1337	C	ALA	1625	18.351	1.116	13.732	1.00	23.64
ATOM	1338	O	ALA	1625	17.135	0.928	13.825	1.00	26.66
ATOM	1339	N	ALA	1626	19.197	0.815	14.712	1.00	21.59
ATOM	1341	CA	ALA	1626	18.708	0.266	15.974	1.00	21.66
ATOM	1342	CB	ALA	1626	19.860	-0.179	16.838	1.00	22.97
ATOM	1343	C	ALA	1626	17.835	1.272	16.731	1.00	24.98
ATOM	1344	O	ALA	1626	17.072	0.891	17.620	1.00	26.84
ATOM	1345	N	ARG	1627	17.978	2.558	16.409	1.00	24.55
ATOM	1347	CA	ARG	1627	17.178	3.598	17.042	1.00	25.29
ATOM	1348	CB	ARG	1627	17.699	4.983	16.673	1.00	26.66
ATOM	1349	CG	ARG	1627	17.675	5.276	15.179	1.00	30.56
ATOM	1350	CD	ARG	1627	18.033	6.715	14.902	1.00	34.97
ATOM	1351	NE	ARG	1627	18.177	6.980	13.470	1.00	40.03
ATOM	1353	CZ	ARG	1627	19.322	6.864	12.809	1.00	40.62
ATOM	1354	NH1	ARG	1627	20.421	6.485	13.441	1.00	46.52
ATOM	1357	NH2	ARG	1627	19.377	7.159	11.523	1.00	43.25
ATOM	1360	C	ARG	1627	15.739				

ATOM	1394	CG1	VAL	1631	12.995	-5.469	23.243	1.00	23.92
ATOM	1395	CG2	VAL	1631	14.197	-3.714	21.895	1.00	24.26
ATOM	1396	C	VAL	1631	10.450	-3.773	22.885	1.00	32.64
ATOM	1397	O	VAL	1631	10.198	-2.821	23.643	1.00	33.01
ATOM	1398	N	THR	1632	9.697	-4.863	22.827	1.00	34.45
ATOM	1400	CA	THR	1632	8.516	-5.035	23.660	1.00	34.29
ATOM	1401	CB	THR	1632	7.466	-5.941	22.962	1.00	34.62
ATOM	1402	OG1	THR	1632	7.965	-7.288	22.881	1.00	34.40
ATOM	1404	CG2	THR	1632	7.154	-5.414	21.551	1.00	31.61
ATOM	1405	C	THR	1632	8.896	-5.678	24.989	1.00	35.41
ATOM	1406	O	THR	1632	10.002	-6.189	25.146	1.00	34.79
ATOM	1407	N	GLU	1633	7.939	-5.706	25.913	1.00	36.86
ATOM	1409	CA	GLU	1633	8.156	-6.298	27.224	1.00	37.27
ATOM	1410	CB	GLU	1633	6.893	-6.182	28.079	1.00	37.66
ATOM	1411	CG	GLU	1633	7.031	-6.718	29.514	1.00	44.43
ATOM	1412	CD	GLU	1633	8.048	-5.959	30.378	1.00	46.68
ATOM	1413	OE1	GLU	1633	8.104	-4.708	30.300	1.00	49.88
ATOM	1414	OE2	GLU	1633	8.783	-6.612	31.156	1.00	48.53
ATOM	1415	C	GLU	1633	8.561	-7.753	27.088	1.00	37.15
ATOM	1416	O	GLU	1633	9.227	-8.292	27.954	1.00	38.60
ATOM	1417	N	ASP	1634	8.167	-8.384	25.990	1.00	38.41
ATOM	1419	CA	ASP	1634	8.505	-9.787	25.770	1.00	38.86
ATOM	1420	CB	ASP	1634	7.381	-10.499	25.013	1.00	44.27
ATOM	1421	CG	ASP	1634	6.022	-10.349	25.690	1.00	50.18
ATOM	1422	OD1	ASP	1634	5.726	-11.141	26.617	1.00	52.07
ATOM	1423	OD2	ASP	1634	5.253	-9.439	25.295	1.00	50.17
ATOM	1424	C	ASP	1634	9.804	-9.947	25.007	1.00	36.23
ATOM	1425	O	ASP	1634	10.141	-11.049	24.608	1.00	35.82
ATOM	1426	N	ASN	1635	10.528	-8.851	24.799	1.00	36.51
ATOM	1428	CA	ASN	1635	11.795	-8.864	24.052	1.00	37.41
ATOM	1429	CB	ASN	1635	12.801	-9.842	24.678	1.00	38.49
ATOM	1430	CG	ASN	1635	13.343	-9.359	26.003	1.00	37.71
ATOM	1431	OD1	ASN	1635	13.499	-8.156	26.227	1.00	38.09
ATOM	1432	ND2	ASN	1635	13.679	-10.300	26.874	1.00	39.63
ATOM	1435	C	ASN	1635	11.655	-9.162	22.552	1.00	36.37
ATOM	1436	O	ASN	1635	12.522	-9.811	21.944	1.00	36.41
ATOM	1437	N	VAL	1636	10.547	-8.721	21.966	1.00	33.79
ATOM	1439	CA	VAL	1636	10.315	-8.910	20.543	1.00	30.59
ATOM	1440	CB	VAL	1636	8.820	-9.139	20.218	1.00	28.83
ATOM	1441	CG1	VAL	1636	8.615	-9.182	18.712	1.00	26.13
ATOM	1442	CG2	VAL	1636	8.339	-10.431	20.838	1.00	25.67
ATOM	1443	C	VAL	1636	10.782	-7.630	19.863	1.00	30.18
ATOM	1444	O	VAL	1636	10.436	-6.527	20.301	1.00	27.86
ATOM	1445	N	MET	1637	11.609	-7.792	18.832	1.00	30.93
ATOM	1447	CA	MET	1637	12.140	-6.679	18.060	1.00	28.34
ATOM	1448	CB	MET	1637	13.397	-7.138	17.330	1.00	30.84
ATOM	1449	CG	MET	1637	14.480	-7.693	18.254	1.00	30.73
ATOM	1450	SD	MET	1637	15.050	-6.490	19.477	1.00	32.20
ATOM	1451	CE	MET	1637	15.074	-7.500	20.938	1.00	28.71
ATOM	1452	C	MET	1637	11.082	-6.264	17.051	1.00	27.29
ATOM	1453	O	MET	1637	10.587	-7.099	16.297	1.00	27.32
ATOM	1454	N	LYS	1638	10.733	-4.983	17.045	1.00	27.19
ATOM	1456	CA	LYS	1638	9.716	-4.450	16.143	1.00	26.38
ATOM	1457	CB	LYS	1638	8.437	-4.120	16.912	1.00	27.09

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ATOM	1458	CG	LYS	1638	7.702	-5.351	17.407	1.00	29.71
ATOM	1459	CD	LYS	1638	6.386	-5.018	18.109	1.00	31.48
ATOM	1460	CE	LYS	1638	5.485	-6.263	18.202	1.00	27.09
ATOM	1461	NZ	LYS	1638	4.888	-6.561	16.869	1.00	26.68
ATOM	1465	C	LYS	1638	10.196	-3.208	15.416	1.00	26.56
ATOM	1466	O	LYS	1638	10.514	-2.194	16.040	1.00	27.40
ATOM	1467	N	ILE	1639	10.211	-3.271	14.092	1.00	24.31
ATOM	1469	CA	ILE	1639	10.649	-2.147	13.289	1.00	24.84
ATOM	1470	CB	ILE	1639	10.924	-2.588	11.836	1.00	25.81
ATOM	1471	CG2	ILE	1639	11.248	-1.395	10.952	1.00	24.18
ATOM	1472	CG1	ILE	1639	12.094	-3.566	11.826	1.00	25.01
ATOM	1473	CD1	ILE	1639	12.075	-4.499	10.675	1.00	27.90
ATOM	1474	C	ILE	1639	9.641	-0.999	13.348	1.00	24.90
ATOM	1475	O	ILE	1639	8.435	-1.186	13.170	1.00	25.24
ATOM	1476	N	ALA	1640	10.167	0.183	13.635	1.00	25.70
ATOM	1478	CA	ALA	1640	9.378	1.392	13.744	1.00	27.61
ATOM	1479	CB	ALA	1640	9.699	2.094	15.070	1.00	26.37
ATOM	1480	C	ALA	1640	9.637	2.348	12.576	1.00	28.35
ATOM	1481	O	ALA	1640	10.650	2.243	11.871	1.00	28.40
ATOM	1482	N	ASP	1641	8.676	3.237	12.354	1.00	29.74
ATOM	1484	CA	ASP	1641	8.760	4.272	11.325	1.00	32.13
ATOM	1485	CB	ASP	1641	9.873	5.273	11.688	1.00	34.31
ATOM	1486	CG	ASP	1641	9.507	6.158	12.896	1.00	36.31
ATOM	1487	OD1	ASP	1641	10.299	7.056	13.258	1.00	42.18
ATOM	1488	OD2	ASP	1641	8.420	5.974	13.483	1.00	41.03
ATOM	1489	C	ASP	1641	8.882	3.840	9.867	1.00	32.00
ATOM	1490	O	ASP	1641	9.339	4.617	9.021	1.00	32.65
ATOM	1491	N	PHE	1642	8.415	2.634	9.563	1.00	30.61
ATOM	1493	CA	PHE	1642	8.473	2.119	8.200	1.00	30.06
ATOM	1494	CB	PHE	1642	8.248	0.606	8.189	1.00	24.46
ATOM	1495	CG	PHE	1642	6.981	0.176	8.854	1.00	23.26
ATOM	1496	CD1	PHE	1642	5.799	0.075	8.125	1.00	19.66
ATOM	1497	CD2	PHE	1642	6.966	-0.134	10.209	1.00	22.88
ATOM	1498	CE1	PHE	1642	4.609	-0.331	8.734	1.00	20.97
ATOM	1499	CE2	PHE	1642	5.785	-0.540	10.830	1.00	26.61
ATOM	1500	CZ	PHE	1642	4.599	-0.639	10.083	1.00	24.82
ATOM	1501	C	PHE	1642	7.512	2.830	7.225	1.00	33.14
ATOM	1502	O	PHE	1642	7.791	2.922	6.029	1.00	36.48
ATOM	1503	N	GLY	1643	6.411	3.372	7.741	1.00	32.65
ATOM	1505	CA	GLY	1643	5.462	4.059	6.876	1.00	32.28
ATOM	1506	C	GLY	1643	5.629	5.560	6.913	1.00	32.19
ATOM	1507	O	GLY	1643	4.795	6.310	6.415	1.00	30.74
ATOM	1508	N	LEU	1644	6.739	5.997	7.486	1.00	36.80
ATOM	1510	CA	LEU	1644	7.052	7.406	7.630	1.00	41.95
ATOM	1511	CB	LEU	1644	8.332	7.551	8.439	1.00	37.41
ATOM	1512	CG	LEU	1644	8.377	8.746	9.369	1.00	38.98
ATOM	1513	CD1	LEU	1644	7.384	8.548	10.493	1.00	40.45
ATOM	1514	CD2	LEU	1644	9.775	8.904	9.929	1.00	41.94
ATOM	1515	C	LEU	1644	7.189	8.150	6.296	1.00	47.55
ATOM	1516	O	LEU	1644	7.787	7.648	5.341	1.00	50.55
ATOM	1517	N	ALA	1645	6.637	9.356	6.247	1.00	52.59
ATOM	1519	CA	ALA	1645	6.686	10.194	5.055	1.00	56.88
ATOM	1520	CB	ALA	1645	5.391	10.999	4.942	1.00	58.01
ATOM	1521	C	ALA	1645	7.880	11.135	5.178	1.00	58.95

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ATOM	1522	O	ALA	1645	8.064	11.770	6.224	1.00	59.37
ATOM	1523	N	ARG	1646	8.700	11.211	4.133	1.00	60.26
ATOM	1525	CA	ARG	1646	9.870	12.088	4.165	1.00	63.04
ATOM	1526	CB	ARG	1646	10.995	11.444	4.976	1.00	64.92
ATOM	1527	C	ARG	1646	10.377	12.461	2.782	1.00	63.84
ATOM	1528	O	ARG	1646	10.361	11.641	1.864	1.00	63.55
ATOM	1529	N	ASP	1647	10.801	13.714	2.633	1.00	65.18
ATOM	1531	CA	ASP	1647	11.332	14.190	1.361	1.00	67.26
ATOM	1532	CB	ASP	1647	10.989	15.670	1.150	1.00	68.92
ATOM	1533	CG	ASP	1647	11.164	16.124	-0.304	1.00	70.88
ATOM	1534	OD1	ASP	1647	12.196	15.811	-0.943	1.00	70.33
ATOM	1535	OD2	ASP	1647	10.258	16.825	-0.808	1.00	71.39
ATOM	1536	C	ASP	1647	12.847	14.005	1.405	1.00	68.40
ATOM	1537	O	ASP	1647	13.545	14.711	2.142	1.00	68.66
ATOM	1538	N	ILE	1648	13.347	13.055	0.621	1.00	68.48
ATOM	1540	CA	ILE	1648	14.777	12.773	0.570	1.00	69.00
ATOM	1541	CB	ILE	1648	15.091	11.535	-0.314	1.00	66.28
ATOM	1542	CG2	ILE	1648	14.231	10.352	0.131	1.00	65.14
ATOM	1543	CG1	ILE	1648	14.869	11.853	-1.799	1.00	63.01
ATOM	1544	CD1	ILE	1648	15.274	10.746	-2.738	1.00	60.11
ATOM	1545	C	ILE	1648	15.542	13.990	0.046	1.00	71.12
ATOM	1546	O	ILE	1648	16.628	14.310	0.525	1.00	72.41
ATOM	1547	N	HIS	1649	14.923	14.710	-0.883	1.00	73.09
ATOM	1549	CA	HIS	1649	15.546	15.890	-1.469	1.00	74.66
ATOM	1550	CB	HIS	1649	14.921	16.191	-2.835	1.00	76.00
ATOM	1551	CG	HIS	1649	15.178	15.157	-3.867	1.00	78.03
ATOM	1552	CD2	HIS	1649	16.314	14.425	-4.151	1.00	78.85
ATOM	1553	ND1	HIS	1649	14.245	14.739	-4.795	1.00	78.49
ATOM	1555	CE1	HIS	1649	14.765	13.835	-5.584	1.00	78.94
ATOM	1556	NE2	HIS	1649	16.005	13.623	-5.226	1.00	78.22
ATOM	1558	C	HIS	1649	15.466	17.108	-0.549	1.00	75.04
ATOM	1559	O	HIS	1649	15.567	18.244	-1.007	1.00	75.49
ATOM	1560	N	HIS	1650	15.265	16.860	0.743	1.00	76.11
ATOM	1562	CA	HIS	1650	15.181	17.918	1.748	1.00	77.63
ATOM	1563	CB	HIS	1650	13.723	18.327	1.995	1.00	81.10
ATOM	1564	CG	HIS	1650	13.206	19.352	1.033	1.00	86.06
ATOM	1565	CD2	HIS	1650	13.662	20.592	0.730	1.00	88.74
ATOM	1566	ND1	HIS	1650	12.099	19.146	0.239	1.00	88.83
ATOM	1568	CE1	HIS	1650	11.893	20.211	-0.511	1.00	90.51
ATOM	1569	NE2	HIS	1650	12.823	21.103	-0.238	1.00	90.75
ATOM	1571	C	HIS	1650	15.824	17.482	3.064	1.00	77.39
ATOM	1572	O	HIS	1650	15.651	18.133	4.091	1.00	77.42
ATOM	1573	N	ILE	1651	16.573	16.385	3.024	1.00	77.73
ATOM	1575	CA	ILE	1651	17.241	15.864	4.212	1.00	77.02
ATOM	1576	CB	ILE	1651	17.788	14.433	3.974	1.00	78.24
ATOM	1577	CG2	ILE	1651	18.647	13.963	5.153	1.00	77.92
ATOM	1578	CG1	ILE	1651	16.633	13.458	3.750	1.00	80.90
ATOM	1579	CD1	ILE	1651	17.094	12.032	3.483	1.00	82.41
ATOM	1580	C	ILE	1651	18.411	16.748	4.620	1.00	76.15
ATOM	1581	O	ILE	1651	19.269	17.078	3.803	1.00	76.52
ATOM	1582	N	ASP	1652	18.432	17.150	5.882	1.00	75.13
ATOM	1584	CA	ASP	1652	19.527	17.957	6.384	1.00	73.91
ATOM	1585	CB	ASP	1652	19.068	18.781	7.592	1.00	76.30
ATOM	1586	CG	ASP	1652	20.216	19.499	8.286	1.00	79.91

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ATOM	1587	OD1	ASP	1652	21.247	19.786	7.636	1.00	82.38
ATOM	1588	OD2	ASP	1652	20.081	19.780	9.497	1.00	81.51
ATOM	1589	C	ASP	1652	20.637	16.984	6.783	1.00	72.31
ATOM	1590	O	ASP	1652	20.599	16.403	7.866	1.00	71.41
ATOM	1591	N	TYR	1653	21.610	16.805	5.894	1.00	71.44
ATOM	1593	CA	TYR	1653	22.736	15.900	6.143	1.00	70.07
ATOM	1594	CB	TYR	1653	23.655	15.849	4.921	1.00	66.96
ATOM	1595	CG	TYR	1653	23.153	14.932	3.834	1.00	66.43
ATOM	1596	CD1	TYR	1653	23.881	14.757	2.657	1.00	66.60
ATOM	1597	CE1	TYR	1653	23.434	13.898	1.653	1.00	68.33
ATOM	1598	CD2	TYR	1653	21.960	14.224	3.981	1.00	66.58
ATOM	1599	CE2	TYR	1653	21.500	13.363	2.990	1.00	68.84
ATOM	1600	CZ	TYR	1653	22.241	13.205	1.823	1.00	69.34
ATOM	1601	OH	TYR	1653	21.781	12.360	0.833	1.00	69.88
ATOM	1603	C	TYR	1653	23.557	16.227	7.391	1.00	70.80
ATOM	1604	O	TYR	1653	24.197	15.351	7.975	1.00	70.62
ATOM	1605	N	TYR	1654	23.531	17.488	7.802	1.00	70.76
ATOM	1607	CA	TYR	1654	24.280	17.902	8.972	1.00	70.97
ATOM	1608	CB	TYR	1654	24.795	19.328	8.783	1.00	69.27
ATOM	1609	CG	TYR	1654	25.935	19.401	7.787	1.00	69.68
ATOM	1610	CD1	TYR	1654	25.696	19.352	6.415	1.00	69.51
ATOM	1611	CE1	TYR	1654	26.750	19.380	5.498	1.00	70.15
ATOM	1612	CD2	TYR	1654	27.256	19.482	8.221	1.00	69.92
ATOM	1613	CE2	TYR	1654	28.314	19.513	7.316	1.00	70.26
ATOM	1614	CZ	TYR	1654	28.057	19.462	5.958	1.00	70.22
ATOM	1615	OH	TYR	1654	29.111	19.492	5.069	1.00	69.67
ATOM	1617	C	TYR	1654	23.503	17.763	10.272	1.00	72.19
ATOM	1618	O	TYR	1654	24.035	18.043	11.344	1.00	73.21
ATOM	1619	N	LYS	1655	22.269	17.275	10.183	1.00	73.05
ATOM	1621	CA	LYS	1655	21.424	17.108	11.363	1.00	74.81
ATOM	1622	CB	LYS	1655	19.955	17.124	10.953	1.00	75.63
ATOM	1623	CG	LYS	1655	18.978	17.239	12.102	1.00	79.16
ATOM	1624	CD	LYS	1655	17.581	17.513	11.576	1.00	84.09
ATOM	1625	CE	LYS	1655	16.517	17.244	12.634	1.00	87.56
ATOM	1626	NZ	LYS	1655	15.139	17.478	12.097	1.00	89.36
ATOM	1630	C	LYS	1655	21.738	15.834	12.156	1.00	75.72
ATOM	1631	O	LYS	1655	21.900	14.751	11.586	1.00	77.14
ATOM	1632	N	LYS	1656	21.815	15.977	13.477	1.00	75.08
ATOM	1634	CA	LYS	1656	22.106	14.857	14.363	1.00	73.36
ATOM	1635	CB	LYS	1656	23.062	15.296	15.477	1.00	72.88
ATOM	1636	CG	LYS	1656	24.475	15.599	15.007	1.00	72.87
ATOM	1637	CD	LYS	1656	25.346	16.048	16.167	1.00	74.66
ATOM	1638	CE	LYS	1656	26.830	15.945	15.828	1.00	74.84
ATOM	1639	NZ	LYS	1656	27.701	16.322	16.981	1.00	73.74
ATOM	1643	C	LYS	1656	20.827	14.311	14.982	1.00	72.45
ATOM	1644	O	LYS	1656	19.795	14.991	15.007	1.00	72.74
ATOM	1645	N	THR	1657	20.900	13.075	15.469	1.00	71.26
ATOM	1647	CA	THR	1657	19.763	12.426	16.107	1.00	70.05
ATOM	1648	CB	THR	1657	19.969	10.886	16.206	1.00	68.30
ATOM	1649	OG1	THR	1657	21.084	10.598	17.060	1.00	69.34
ATOM	1651	CG2	THR	1657	20.244	10.292	14.839	1.00	66.16
ATOM	1652	C	THR	1657	19.707	13.019	17.504	1.00	70.37
ATOM	1653	O	THR	1657	20.608	13.761	17.892	1.00	71.47
ATOM	1654	N	THR	1658	18.669	12.691	18.263	1.00	70.80

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ATOM	1656	CA	THR	1658	18.559	13.205	19.626	1.00	71.54
ATOM	1657	CB	THR	1658	17.334	12.600	20.325	1.00	71.20
ATOM	1658	C	THR	1658	19.844	12.865	20.394	1.00	70.91
ATOM	1659	O	THR	1658	20.429	13.722	21.063	1.00	71.25
ATOM	1660	N	ASN	1659	20.331	11.639	20.199	1.00	68.87
ATOM	1662	CA	ASN	1659	21.537	11.157	20.871	1.00	65.52
ATOM	1663	CB	ASN	1659	21.602	9.635	20.796	1.00	67.39
ATOM	1664	CG	ASN	1659	22.419	9.032	21.916	1.00	69.42
ATOM	1665	OD1	ASN	1659	22.261	9.410	23.076	1.00	71.70
ATOM	1666	ND2	ASN	1659	23.278	8.069	21.583	1.00	68.93
ATOM	1669	C	ASN	1659	22.830	11.749	20.318	1.00	62.51
ATOM	1670	O	ASN	1659	23.917	11.351	20.733	1.00	61.47
ATOM	1671	N	GLY	1660	22.706	12.654	19.348	1.00	59.76
ATOM	1673	CA	GLY	1660	23.859	13.307	18.750	1.00	57.70
ATOM	1674	C	GLY	1660	24.553	12.593	17.597	1.00	56.98
ATOM	1675	O	GLY	1660	25.659	12.979	17.199	1.00	57.55
ATOM	1676	N	ARG	1661	23.909	11.573	17.037	1.00	55.34
ATOM	1678	CA	ARG	1661	24.504	10.826	15.928	1.00	52.28
ATOM	1679	CB	ARG	1661	24.255	9.334	16.092	1.00	50.68
ATOM	1680	CG	ARG	1661	24.811	8.744	17.365	1.00	49.61
ATOM	1681	CD	ARG	1661	24.542	7.267	17.361	1.00	52.30
ATOM	1682	NE	ARG	1661	24.942	6.599	18.595	1.00	53.64
ATOM	1684	CZ	ARG	1661	24.731	5.306	18.826	1.00	56.32
ATOM	1685	NH1	ARG	1661	24.124	4.559	17.901	1.00	54.04
ATOM	1688	NH2	ARG	1661	25.145	4.754	19.965	1.00	54.48
ATOM	1691	C	ARG	1661	24.015	11.288	14.560	1.00	49.89
ATOM	1692	O	ARG	1661	22.916	11.812	14.429	1.00	51.43
ATOM	1693	N	LEU	1662	24.839	11.080	13.542	1.00	45.78
ATOM	1695	CA	LEU	1662	24.503	11.481	12.186	1.00	43.05
ATOM	1696	CB	LEU	1662	25.762	12.020	11.492	1.00	42.15
ATOM	1697	CG	LEU	1662	26.351	13.306	12.088	1.00	40.60
ATOM	1698	CD1	LEU	1662	27.780	13.512	11.641	1.00	38.14
ATOM	1699	CD2	LEU	1662	25.484	14.499	11.705	1.00	42.00
ATOM	1700	C	LEU	1662	23.867	10.346	11.370	1.00	41.81
ATOM	1701	O	LEU	1662	24.548	9.406	10.957	1.00	40.46
ATOM	1702	N	PRO	1663	22.546	10.428	11.118	1.00	40.49
ATOM	1703	CD	PRO	1663	21.659	11.519	11.561	1.00	40.60
ATOM	1704	CA	PRO	1663	21.794	9.423	10.351	1.00	38.17
ATOM	1705	CB	PRO	1663	20.433	10.095	10.158	1.00	38.43
ATOM	1706	CG	PRO	1663	20.282	10.901	11.414	1.00	40.65
ATOM	1707	C	PRO	1663	22.445	9.059	9.012	1.00	35.40
ATOM	1708	O	PRO	1663	22.265	7.949	8.521	1.00	33.01
ATOM	1709	N	VAL	1664	23.200	9.989	8.426	1.00	34.56
ATOM	1711	CA	VAL	1664	23.889	9.722	7.160	1.00	32.91
ATOM	1712	CB	VAL	1664	24.757	10.916	6.659	1.00	33.13
ATOM	1713	CG1	VAL	1664	23.912	11.929	5.968	1.00	33.44
ATOM	1714	CG2	VAL	1664	25.521	11.554	7.792	1.00	33.68
ATOM	1715	C	VAL	1664	24.812	8.511	7.266	1.00	30.58
ATOM	1716	O	VAL	1664	25.157	7.903	6.257	1.00	29.20
ATOM	1717	N	LYS	1665	25.211	8.171	8.489	1.00	28.02
ATOM	1719	CA	LYS	1665	26.102	7.044	8.726	1.00	24.95
ATOM	1720	CB	LYS	1665	26.749	7.153	10.098	1.00	24.39
ATOM	1721	CG	LYS	1665	27.811	8.231	10.140	1.00	28.36
ATOM	1722	CD	LYS	1665	28.189	8.628	11.548	1.00	29.24

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ATOM	1723	CE	LYS	1665	29.269	9.690	11.489	1.00	31.15
ATOM	1724	NZ	LYS	1665	29.639	10.194	12.836	1.00	35.47
ATOM	1728	C	LYS	1665	25.440	5.692	8.543	1.00	25.16
ATOM	1729	O	LYS	1665	26.096	4.671	8.627	1.00	24.34
ATOM	1730	N	TRP	1666	24.138	5.698	8.286	1.00	25.16
ATOM	1732	CA	TRP	1666	23.414	4.461	8.053	1.00	26.61
ATOM	1733	CB	TRP	1666	22.157	4.412	8.917	1.00	28.17
ATOM	1734	CG	TRP	1666	22.428	3.931	10.330	1.00	30.26
ATOM	1735	CD2	TRP	1666	22.930	4.714	11.426	1.00	26.92
ATOM	1736	CE2	TRP	1666	23.063	3.837	12.537	1.00	26.34
ATOM	1737	CE3	TRP	1666	23.286	6.057	11.598	1.00	24.69
ATOM	1738	CD1	TRP	1666	22.276	2.656	10.800	1.00	26.44
ATOM	1739	NE1	TRP	1666	22.659	2.592	12.118	1.00	25.65
ATOM	1741	CZ2	TRP	1666	23.535	4.264	13.779	1.00	24.97
ATOM	1742	CZ3	TRP	1666	23.758	6.484	12.837	1.00	22.23
ATOM	1743	CH2	TRP	1666	23.877	5.587	13.908	1.00	24.97
ATOM	1744	C	TRP	1666	23.048	4.345	6.572	1.00	27.24
ATOM	1745	O	TRP	1666	22.573	3.301	6.116	1.00	29.16
ATOM	1746	N	MET	1667	23.355	5.390	5.811	1.00	26.70
ATOM	1748	CA	MET	1667	23.022	5.444	4.398	1.00	25.21
ATOM	1749	CB	MET	1667	22.828	6.893	3.963	1.00	28.81
ATOM	1750	CG	MET	1667	21.704	7.630	4.637	1.00	35.42
ATOM	1751	SD	MET	1667	21.567	9.283	3.924	1.00	42.64
ATOM	1752	CE	MET	1667	20.959	8.858	2.369	1.00	41.32
ATOM	1753	C	MET	1667	23.984	4.807	3.417	1.00	25.03
ATOM	1754	O	MET	1667	25.182	5.047	3.446	1.00	24.24
ATOM	1755	N	ALA	1668	23.420	4.034	2.501	1.00	26.70
ATOM	1757	CA	ALA	1668	24.186	3.398	1.441	1.00	27.82
ATOM	1758	CB	ALA	1668	23.272	2.509	0.601	1.00	25.36
ATOM	1759	C	ALA	1668	24.738	4.528	0.575	1.00	28.42
ATOM	1760	O	ALA	1668	24.044	5.521	0.321	1.00	27.52
ATOM	1761	N	PRO	1669	25.972	4.374	0.065	1.00	28.95
ATOM	1762	CD	PRO	1669	26.867	3.214	0.170	1.00	27.98
ATOM	1763	CA	PRO	1669	26.571	5.418	-0.775	1.00	28.76
ATOM	1764	CB	PRO	1669	27.814	4.731	-1.326	1.00	28.58
ATOM	1765	CG	PRO	1669	28.193	3.809	-0.209	1.00	30.22
ATOM	1766	C	PRO	1669	25.647	5.909	-1.893	1.00	27.08
ATOM	1767	O	PRO	1669	25.496	7.107	-2.093	1.00	28.31
ATOM	1768	N	GLU	1670	24.993	4.997	-2.595	1.00	25.42
ATOM	1770	CA	GLU	1670	24.110	5.423	-3.673	1.00	27.02
ATOM	1771	CB	GLU	1670	23.680	4.233	-4.542	1.00	27.18
ATOM	1772	CG	GLU	1670	22.662	3.294	-3.911	1.00	27.66
ATOM	1773	CD	GLU	1670	23.280	2.162	-3.112	1.00	27.75
ATOM	1774	OE1	GLU	1670	22.488	1.309	-2.647	1.00	27.12
ATOM	1775	OE2	GLU	1670	24.526	2.114	-2.944	1.00	21.64
ATOM	1776	C	GLU	1670	22.896	6.229	-3.189	1.00	26.88
ATOM	1777	O	GLU	1670	22.348	7.037	-3.929	1.00	24.52
ATOM	1778	N	ALA	1671	22.477	6.009	-1.948	1.00	29.43
ATOM	1780	CA	ALA	1671	21.342	6.744	-1.392	1.00	29.29
ATOM	1781	CB	ALA	1671	20.751	5.989	-0.217	1.00	26.98
ATOM	1782	C	ALA	1671	21.826	8.124	-0.939	1.00	31.14
ATOM	1783	O	ALA	1671	21.159	9.135	-1.143	1.00	31.67
ATOM	1784	N	LEU	1672	23.013	8.139	-0.343	1.00	32.31
ATOM	1786	CA	LEU	1672	23.636	9.352	0.154	1.00	33.79

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ATOM	1787	CB	LEU	1672	24.841				
ATOM	1788	CG	LEU	1672	25.585	8.986	1.008	1.00	34.49
ATOM	1789	CD1	LEU	1672	24.713	10.166	1.618	1.00	37.16
ATOM	1790	CD2	LEU	1672	26.863	10.840	2.666	1.00	42.22
ATOM	1791	C	LEU	1672	24.078	9.665	2.237	1.00	33.93
ATOM	1792	O	LEU	1672	23.789	10.280	-0.972	1.00	36.30
ATOM	1793	N	PHE	1673	24.770	11.478	-0.949	1.00	39.09
ATOM	1795	CA	PHE	1673	25.266	9.723	-1.957	1.00	34.39
ATOM	1796	CB	PHE	1673	26.553	10.504	-3.075	1.00	33.81
ATOM	1797	CG	PHE	1673	27.661	9.874	-3.625	1.00	33.15
ATOM	1798	CD1	PHE	1673	28.313	9.761	-2.617	1.00	33.44
ATOM	1799	CD2	PHE	1673	28.055	8.545	-2.419	1.00	32.17
ATOM	1800	CE1	PHE	1673	29.346	10.867	-1.861	1.00	34.87
ATOM	1801	CE2	PHE	1673	29.090	8.419	-1.484	1.00	31.98
ATOM	1802	CZ	PHE	1673	29.736	10.757	-0.919	1.00	36.31
ATOM	1803	C	PHE	1673	24.273	9.525	-0.732	1.00	34.55
ATOM	1804	O	PHE	1673	24.135	10.670	-4.217	1.00	34.79
ATOM	1805	N	ASP	1674	23.584	11.754	-4.765	1.00	35.74
ATOM	1807	CA	ASP	1674	22.650	9.588	-4.572	1.00	37.31
ATOM	1808	CB	ASP	1674	22.917	9.601	-5.698	1.00	35.61
ATOM	1809	CG	ASP	1674	24.362	8.392	-6.600	1.00	37.01
ATOM	1810	OD1	ASP	1674	25.030	8.288	-7.041	1.00	41.02
ATOM	1811	OD2	ASP	1674	24.828	9.340	-7.194	1.00	43.07
ATOM	1812	C	ASP	1674	21.162	7.145	-7.251	1.00	42.24
ATOM	1813	O	ASP	1674	20.315	9.632	-5.360	1.00	37.06
ATOM	1814	N	ARG	1675	20.840	9.506	-6.257	1.00	36.37
ATOM	1816	CA	ARG	1675	19.445	9.745	-4.077	1.00	37.78
ATOM	1817	CB	ARG	1675	18.832	9.791	-3.650	1.00	39.41
ATOM	1818	CG	ARG	1675	19.413	11.137	-4.039	1.00	44.39
ATOM	1819	CD	ARG	1675	19.516	12.299	-3.269	1.00	54.30
ATOM	1820	NE	ARG	1675	20.060	13.551	-4.127	1.00	63.84
ATOM	1822	CZ	ARG	1675	19.652	14.664	-3.349	1.00	73.69
ATOM	1823	NH1	ARG	1675	18.695	15.925	-3.453	1.00	77.10
ATOM	1826	NH2	ARG	1675	20.177	16.253	-4.312	1.00	79.65
ATOM	1829	C	ARG	1675	18.617	16.855	-2.665	1.00	79.31
ATOM	1830	O	ARG	1675	17.447	8.639	-4.221	1.00	37.46
ATOM	1831	N	ILE	1676	19.235	8.808	-4.557	1.00	38.57
ATOM	1833	CA	ILE	1676	18.545	7.475	-4.351	1.00	34.37
ATOM	1834	CB	ILE	1676	19.358	6.313	-4.874	1.00	32.99
ATOM	1835	CG2	ILE	1676	18.552	5.644	-5.976	1.00	33.98
ATOM	1836	CG1	ILE	1676	19.708	4.529	-6.602	1.00	35.04
ATOM	1837	CD1	ILE	1676	20.799	6.663	-7.050	1.00	34.92
ATOM	1838	C	ILE	1676	18.315	6.200	-7.962	1.00	41.16
ATOM	1839	O	ILE	1676	19.245	5.315	-3.743	1.00	31.55
ATOM	1840	N	TYR	1677	17.082	4.632	-3.300	1.00	30.65
ATOM	1842	CA	TYR	1677	16.701	5.279	-3.246	1.00	30.88
ATOM	1843	CB	TYR	1677	15.771	4.371	-2.173	1.00	27.10
ATOM	1844	CG	TYR	1677	16.457	5.074	-1.208	1.00	28.30
ATOM	1845	CD1	TYR	1677	16.598	6.136	-0.406	1.00	30.61
ATOM	1846	CE1	TYR	1677	17.212	7.432	-0.905	1.00	30.82
ATOM	1847	CD2	TYR	1677	16.952	8.424	-0.159	1.00	30.75
ATOM	1848	CE2	TYR	1677	17.567	5.857	0.863	1.00	29.75
ATOM	1849	CZ	TYR	1677	17.688	6.842	1.621	1.00	32.62
ATOM	1850	OH	TYR	1677	18.238	8.125	1.110	1.00	34.51
						9.118	1.888	1.00	38.89

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ATOM	1852	C	TYR	1677	16.029	3.149	-2.743	1.00	25.47
ATOM	1853	O	TYR	1677	15.132	3.264	-3.578	1.00	26.00
ATOM	1854	N	THR	1678	16.459	1.983	-2.272	1.00	24.27
ATOM	1856	CA	THR	1678	15.942	0.701	-2.734	1.00	24.09
ATOM	1857	CB	THR	1678	16.830	0.123	-3.853	1.00	24.19
ATOM	1858	OG1	THR	1678	18.165	-0.008	-3.349	1.00	27.81
ATOM	1860	CG2	THR	1678	16.843	1.009	-5.085	1.00	24.15
ATOM	1861	C	THR	1678	15.979	-0.297	-1.577	1.00	25.02
ATOM	1862	O	THR	1678	16.379	0.036	-0.465	1.00	27.65
ATOM	1863	N	HIS	1679	15.569	-1.530	-1.844	1.00	25.04
ATOM	1865	CA	HIS	1679	15.591	-2.560	-0.818	1.00	24.35
ATOM	1866	CB	HIS	1679	14.853	-3.812	-1.298	1.00	23.78
ATOM	1867	CG	HIS	1679	13.390	-3.592	-1.536	1.00	27.24
ATOM	1868	CD2	HIS	1679	12.627	-3.758	-2.643	1.00	28.22
ATOM	1869	ND1	HIS	1679	12.532	-3.137	-0.551	1.00	30.64
ATOM	1871	CE1	HIS	1679	11.310	-3.028	-1.041	1.00	28.13
ATOM	1872	NE2	HIS	1679	11.339	-3.400	-2.307	1.00	28.52
ATOM	1874	C	HIS	1679	17.056	-2.846	-0.514	1.00	22.52
ATOM	1875	O	HIS	1679	17.419	-3.179	0.613	1.00	22.58
ATOM	1876	N	GLN	1680	17.898	-2.604	-1.516	1.00	24.34
ATOM	1878	CA	GLN	1680	19.341	-2.800	-1.406	1.00	23.52
ATOM	1879	CB	GLN	1680	19.998	-2.781	-2.782	1.00	25.36
ATOM	1880	CG	GLN	1680	19.741	-4.050	-3.577	1.00	33.28
ATOM	1881	CD	GLN	1680	19.212	-3.763	-4.949	1.00	34.68
ATOM	1882	OE1	GLN	1680	18.683	-2.686	-5.187	1.00	41.24
ATOM	1883	NE2	GLN	1680	19.357	-4.713	-5.867	1.00	32.10
ATOM	1886	C	GLN	1680	19.998	-1.767	-0.514	1.00	23.38
ATOM	1887	O	GLN	1680	20.925	-2.094	0.224	1.00	25.12
ATOM	1888	N	SER	1681	19.533	-0.521	-0.562	1.00	20.87
ATOM	1890	CA	SER	1681	20.133	0.480	0.303	1.00	20.53
ATOM	1891	CB	SER	1681	19.821	1.919	-0.151	1.00	19.58
ATOM	1892	OG	SER	1681	18.445	2.126	-0.425	1.00	20.67
ATOM	1894	C	SER	1681	19.696	0.189	1.741	1.00	22.22
ATOM	1895	O	SER	1681	20.439	0.455	2.681	1.00	23.62
ATOM	1896	N	ASP	1682	18.530	-0.436	1.900	1.00	22.44
ATOM	1898	CA	ASP	1682	18.054	-0.816	3.231	1.00	22.70
ATOM	1899	CB	ASP	1682	16.607	-1.293	3.180	1.00	24.24
ATOM	1900	CG	ASP	1682	15.603	-0.165	3.352	1.00	28.23
ATOM	1901	OD1	ASP	1682	14.410	-0.425	3.108	1.00	28.14
ATOM	1902	OD2	ASP	1682	15.976	0.960	3.757	1.00	25.23
ATOM	1903	C	ASP	1682	18.926	-1.941	3.777	1.00	23.92
ATOM	1904	O	ASP	1682	19.121	-2.057	4.990	1.00	26.24
ATOM	1905	N	VAL	1683	19.433	-2.788	2.884	1.00	23.67
ATOM	1907	CA	VAL	1683	20.300	-3.888	3.302	1.00	22.42
ATOM	1908	CB	VAL	1683	20.562	-4.881	2.141	1.00	23.70
ATOM	1909	CG1	VAL	1683	21.724	-5.802	2.459	1.00	19.73
ATOM	1910	CG2	VAL	1683	19.292	-5.713	1.889	1.00	19.85
ATOM	1911	C	VAL	1683	21.584	-3.298	3.860	1.00	21.94
ATOM	1912	O	VAL	1683	22.030	-3.688	4.938	1.00	22.69
ATOM	1913	N	TRP	1684	22.141	-2.320	3.154	1.00	20.51
ATOM	1915	CA	TRP	1684	23.349	-1.633	3.611	1.00	20.31
ATOM	1916	CB	TRP	1684	23.659	-0.446	2.680	1.00	19.01
ATOM	1917	CG	TRP	1684	24.802	0.410	3.145	1.00	20.67
ATOM	1918	CD2	TRP	1684	26.114	0.468	2.587	1.00	22.26

ATOM	1919	CE2	TRP	1684	26.890	1.316	3.408	1.00	21.22
ATOM	1920	CE3	TRP	1684	26.718	-0.127	1.463	1.00	22.51
ATOM	1921	CD1	TRP	1684	24.825	1.229	4.248	1.00	19.91
ATOM	1922	NE1	TRP	1684	26.079	1.763	4.414	1.00	18.59
ATOM	1924	CZ2	TRP	1684	28.236	1.586	3.148	1.00	20.81
ATOM	1925	CZ3	TRP	1684	28.059	0.141	1.204	1.00	22.01
ATOM	1926	CH2	TRP	1684	28.806	0.992	2.047	1.00	23.34
ATOM	1927	C	TRP	1684	23.131	-1.150	5.069	1.00	21.49
ATOM	1928	O	TRP	1684	23.958	-1.412	5.954	1.00	23.34
ATOM	1929	N	SER	1685	22.015	-0.463	5.308	1.00	21.84
ATOM	1931	CA	SER	1685	21.652	0.042	6.634	1.00	20.02
ATOM	1932	CB	SER	1685	20.310	0.773	6.559	1.00	19.12
ATOM	1933	OG	SER	1685	20.335	1.791	5.578	1.00	21.62
ATOM	1935	C	SER	1685	21.551	-1.111	7.648	1.00	22.64
ATOM	1936	O	SER	1685	21.908	-0.946	8.829	1.00	22.09
ATOM	1937	N	PHE	1686	21.043	-2.266	7.202	1.00	22.44
ATOM	1939	CA	PHE	1686	20.939	-3.438	8.075	1.00	22.91
ATOM	1940	CB	PHE	1686	20.196	-4.588	7.380	1.00	23.75
ATOM	1941	CG	PHE	1686	20.027	-5.808	8.256	1.00	23.61
ATOM	1942	CD1	PHE	1686	19.220	-5.757	9.388	1.00	21.21
ATOM	1943	CD2	PHE	1686	20.731	-6.976	7.990	1.00	23.91
ATOM	1944	CE1	PHE	1686	19.118	-6.836	10.240	1.00	20.66
ATOM	1945	CE2	PHE	1686	20.636	-8.074	8.841	1.00	22.47
ATOM	1946	CZ	PHE	1686	19.828	-7.999	9.972	1.00	23.35
ATOM	1947	C	PHE	1686	22.339	-3.904	8.522	1.00	22.60
ATOM	1948	O	PHE	1686	22.526	-4.382	9.646	1.00	22.83
ATOM	1949	N	GLY	1687	23.312	-3.770	7.626	1.00	23.82
ATOM	1951	CA	GLY	1687	24.682	-4.140	7.941	1.00	22.58
ATOM	1952	C	GLY	1687	25.175	-3.262	9.071	1.00	21.49
ATOM	1953	O	GLY	1687	25.832	-3.749	9.990	1.00	21.62
ATOM	1954	N	VAL	1688	24.849	-1.968	9.008	1.00	21.15
ATOM	1956	CA	VAL	1688	25.229	-1.008	10.052	1.00	20.56
ATOM	1957	CB	VAL	1688	24.894	0.479	9.647	1.00	17.69
ATOM	1958	CG1	VAL	1688	25.408	1.456	10.690	1.00	15.11
ATOM	1959	CG2	VAL	1688	25.518	0.821	8.314	1.00	11.54
ATOM	1960	C	VAL	1688	24.494	-1.398	11.346	1.00	22.60
ATOM	1961	O	VAL	1688	25.083	-1.407	12.428	1.00	25.23
ATOM	1962	N	LEU	1689	23.215	-1.755	11.229	1.00	26.09
ATOM	1964	CA	LEU	1689	22.423	-2.175	12.387	1.00	25.16
ATOM	1965	CB	LEU	1689	20.976	-2.455	11.965	1.00	25.91
ATOM	1966	CG	LEU	1689	19.913	-2.560	13.068	1.00	27.54
ATOM	1967	CD1	LEU	1689	18.557	-2.241	12.496	1.00	28.11
ATOM	1968	CD2	LEU	1689	19.898	-3.940	13.704	1.00	31.67
ATOM	1969	C	LEU	1689	23.055	-3.426	13.018	1.00	27.49
ATOM	1970	O	LEU	1689	23.128	-3.532	14.246	1.00	28.99
ATOM	1971	N	LEU	1690	23.485	-4.374	12.180	1.00	27.67
ATOM	1973	CA	LEU	1690	24.149	-5.596	12.643	1.00	26.76
ATOM	1974	CB	LEU	1690	24.616	-6.453	11.456	1.00	28.58
ATOM	1975	CG	LEU	1690	23.651	-7.406	10.733	1.00	29.46
ATOM	1976	CD1	LEU	1690	24.372	-8.064	9.565	1.00	27.79
ATOM	1977	CD2	LEU	1690	23.130	-8.488	11.691	1.00	28.15
ATOM	1978	C	LEU	1690	25.362	-5.176	13.476	1.00	26.19
ATOM	1979	O	LEU	1690	25.565	-5.670	14.597	1.00	25.29
ATOM	1980	N	TRP	1691	26.124	-4.217	12.946	1.00	25.89

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ATOM	1982	CA	TRP	1691	27.302	-3.682	13.631	1.00	27.31
ATOM	1983	CB	TRP	1691	27.979	-2.628	12.755	1.00	25.21
ATOM	1984	CG	TRP	1691	29.338	-2.170	13.257	1.00	27.00
ATOM	1985	CD2	TRP	1691	29.606	-1.060	14.134	1.00	24.28
ATOM	1986	CE2	TRP	1691	31.001	-0.988	14.297	1.00	23.03
ATOM	1987	CE3	TRP	1691	28.792	-0.118	14.778	1.00	22.80
ATOM	1988	CD1	TRP	1691	30.562	-2.712	12.944	1.00	24.10
ATOM	1989	NE1	TRP	1691	31.557	-2.010	13.567	1.00	23.41
ATOM	1991	CZ2	TRP	1691	31.617	-0.011	15.097	1.00	25.00
ATOM	1992	CZ3	TRP	1691	29.398	0.851	15.573	1.00	26.78
ATOM	1993	CH2	TRP	1691	30.802	0.900	15.719	1.00	27.78
ATOM	1994	C	TRP	1691	26.947	-3.088	15.012	1.00	28.70
ATOM	1995	O	TRP	1691	27.708	-3.245	15.974	1.00	29.56
ATOM	1996	N	GLU	1692	25.808	-2.400	15.104	1.00	29.51
ATOM	1998	CA	GLU	1692	25.349	-1.817	16.371	1.00	27.55
ATOM	1999	CB	GLU	1692	24.120	-0.935	16.171	1.00	28.35
ATOM	2000	CG	GLU	1692	24.273	0.221	15.219	1.00	24.70
ATOM	2001	CD	GLU	1692	22.982	0.989	15.100	1.00	25.44
ATOM	2002	OE1	GLU	1692	22.224	0.744	14.148	1.00	24.34
ATOM	2003	OE2	GLU	1692	22.696	1.816	15.982	1.00	27.57
ATOM	2004	C	GLU	1692	24.958	-2.918	17.352	1.00	28.74
ATOM	2005	O	GLU	1692	25.099	-2.753	18.557	1.00	28.76
ATOM	2006	N	ILE	1693	24.421	-4.023	16.844	1.00	29.23
ATOM	2008	CA	ILE	1693	24.027	-5.125	17.712	1.00	27.48
ATOM	2009	CB	ILE	1693	23.205	-6.226	16.944	1.00	26.80
ATOM	2010	CG2	ILE	1693	22.983	-7.469	17.842	1.00	22.98
ATOM	2011	CG1	ILE	1693	21.840	-5.658	16.508	1.00	27.36
ATOM	2012	CD1	ILE	1693	21.005	-6.585	15.635	1.00	24.84
ATOM	2013	C	ILE	1693	25.259	-5.750	18.357	1.00	27.27
ATOM	2014	O	ILE	1693	25.320	-5.902	19.575	1.00	28.15
ATOM	2015	N	PHE	1694	26.273	-6.043	17.552	1.00	27.83
ATOM	2017	CA	PHE	1694	27.473	-6.677	18.095	1.00	29.88
ATOM	2018	CB	PHE	1694	28.143	-7.525	17.011	1.00	28.66
ATOM	2019	CG	PHE	1694	27.223	-8.574	16.463	1.00	29.92
ATOM	2020	CD1	PHE	1694	26.628	-8.424	15.220	1.00	30.20
ATOM	2021	CD2	PHE	1694	26.809	-9.630	17.269	1.00	30.81
ATOM	2022	CE1	PHE	1694	25.625	-9.294	14.801	1.00	32.42
ATOM	2023	CE2	PHE	1694	25.805	-10.508	16.857	1.00	32.30
ATOM	2024	CZ	PHE	1694	25.210	-10.337	15.628	1.00	31.13
ATOM	2025	C	PHE	1694	28.429	-5.784	18.890	1.00	31.07
ATOM	2026	O	PHE	1694	29.376	-6.273	19.509	1.00	33.16
ATOM	2027	N	THR	1695	28.157	-4.480	18.897	1.00	29.20
ATOM	2029	CA	THR	1695	28.934	-3.532	19.670	1.00	27.38
ATOM	2030	CB	THR	1695	29.412	-2.333	18.823	1.00	24.77
ATOM	2031	OG1	THR	1695	28.287	-1.652	18.274	1.00	26.27
ATOM	2033	CG2	THR	1695	30.305	-2.800	17.706	1.00	20.18
ATOM	2034	C	THR	1695	28.053	-3.034	20.822	1.00	29.84
ATOM	2035	O	THR	1695	28.430	-2.103	21.548	1.00	32.77
ATOM	2036	N	LEU	1696	26.898	-3.687	20.988	1.00	28.52
ATOM	2038	CA	LEU	1696	25.915	-3.364	22.029	1.00	28.82
ATOM	2039	CB	LEU	1696	26.356	-3.886	23.394	1.00	32.50
ATOM	2040	CG	LEU	1696	26.658	-5.379	23.476	1.00	33.24
ATOM	2041	CD1	LEU	1696	27.205	-5.717	24.849	1.00	34.15
ATOM	2042	CD2	LEU	1696	25.398	-6.150	23.191	1.00	37.24

ATOM	2043	C	LEU	1696	25.553	-1.888	22.131	1.00	26.98
ATOM	2044	O	LEU	1696	25.579	-1.297	23.207	1.00	27.59
ATOM	2045	N	GLY	1697	25.148	-1.317	21.007	1.00	27.86
ATOM	2047	CA	GLY	1697	24.767	0.074	20.980	1.00	27.40
ATOM	2048	C	GLY	1697	25.927	0.962	20.618	1.00	27.47
ATOM	2049	O	GLY	1697	25.957	2.132	20.998	1.00	28.78
ATOM	2050	N	GLY	1698	26.888	0.416	19.885	1.00	27.26
ATOM	2052	CA	GLY	1698	28.031	1.212	19.482	1.00	29.54
ATOM	2053	C	GLY	1698	27.651	2.301	18.492	1.00	31.17
ATOM	2054	O	GLY	1698	26.669	2.177	17.755	1.00	33.73
ATOM	2055	N	SER	1699	28.418	3.380	18.481	1.00	29.96
ATOM	2057	CA	SER	1699	28.168	4.491	17.577	1.00	29.37
ATOM	2058	CB	SER	1699	28.438	5.810	18.319	1.00	31.77
ATOM	2059	OG	SER	1699	28.575	6.919	17.431	1.00	38.42
ATOM	2061	C	SER	1699	29.093	4.350	16.369	1.00	27.98
ATOM	2062	O	SER	1699	30.299	4.310	16.529	1.00	28.18
ATOM	2063	N	PRO	1700	28.537	4.240	15.153	1.00	29.62
ATOM	2064	CD	PRO	1700	27.104	4.259	14.794	1.00	31.22
ATOM	2065	CA	PRO	1700	29.381	4.107	13.958	1.00	28.95
ATOM	2066	CB	PRO	1700	28.356	4.003	12.807	1.00	27.21
ATOM	2067	CG	PRO	1700	27.095	3.556	13.460	1.00	29.33
ATOM	2068	C	PRO	1700	30.205	5.379	13.773	1.00	28.78
ATOM	2069	O	PRO	1700	29.737	6.469	14.110	1.00	30.04
ATOM	2070	N	TYR	1701	31.426	5.239	13.264	1.00	28.35
ATOM	2072	CA	TYR	1701	32.296	6.390	12.987	1.00	30.77
ATOM	2073	CB	TYR	1701	31.921	6.987	11.615	1.00	31.67
ATOM	2074	CG	TYR	1701	32.060	6.037	10.454	1.00	34.61
ATOM	2075	CD1	TYR	1701	30.952	5.673	9.686	1.00	38.26
ATOM	2076	CE1	TYR	1701	31.083	4.806	8.587	1.00	40.99
ATOM	2077	CD2	TYR	1701	33.301	5.520	10.106	1.00	38.16
ATOM	2078	CE2	TYR	1701	33.449	4.662	9.020	1.00	41.04
ATOM	2079	CZ	TYR	1701	32.343	4.312	8.263	1.00	43.11
ATOM	2080	OH	TYR	1701	32.531	3.478	7.181	1.00	49.53
ATOM	2082	C	TYR	1701	32.305	7.532	14.029	1.00	31.41
ATOM	2083	O	TYR	1701	32.026	8.689	13.698	1.00	33.59
ATOM	2084	N	PRO	1702	32.635	7.230	15.296	1.00	30.92
ATOM	2085	CD	PRO	1702	32.998	5.938	15.888	1.00	32.30
ATOM	2086	CA	PRO	1702	32.656	8.283	16.314	1.00	30.05
ATOM	2087	CB	PRO	1702	33.123	7.548	17.561	1.00	27.77
ATOM	2088	CG	PRO	1702	32.676	6.174	17.338	1.00	32.34
ATOM	2089	C	PRO	1702	33.659	9.366	15.944	1.00	31.42
ATOM	2090	O	PRO	1702	34.769	9.055	15.513	1.00	30.95
ATOM	2091	N	GLY	1703	33.257	10.627	16.117	1.00	31.30
ATOM	2093	CA	GLY	1703	34.122	11.751	15.817	1.00	29.66
ATOM	2094	C	GLY	1703	34.172	12.138	14.351	1.00	31.00
ATOM	2095	O	GLY	1703	34.752	13.165	13.999	1.00	30.69
ATOM	2096	N	VAL	1704	33.551	11.331	13.491	1.00	31.11
ATOM	2098	CA	VAL	1704	33.553	11.610	12.059	1.00	29.88
ATOM	2099	CB	VAL	1704	33.539	10.310	11.244	1.00	28.41
ATOM	2100	CG1	VAL	1704	33.585	10.624	9.750	1.00	26.24
ATOM	2101	CG2	VAL	1704	34.702	9.429	11.649	1.00	24.10
ATOM	2102	C	VAL	1704	32.396	12.508	11.604	1.00	30.80
ATOM	2103	O	VAL	1704	31.224	12.146	11.712	1.00	32.50
ATOM	2104	N	PRO	1705	32.718	13.705	11.104	1.00	30.86

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ATOM	2105	CD	PRO	1705	34.039	14.350	11.077	1.00	30.59
ATOM	2106	CA	PRO	1705	31.682	14.625	10.645	1.00	31.47
ATOM	2107	CB	PRO	1705	32.400	15.971	10.680	1.00	32.75
ATOM	2108	CG	PRO	1705	33.774	15.607	10.289	1.00	32.59
ATOM	2109	C	PRO	1705	31.258	14.264	9.239	1.00	32.19
ATOM	2110	O	PRO	1705	31.974	13.536	8.549	1.00	33.91
ATOM	2111	N	VAL	1706	30.124	14.814	8.806	1.00	32.57
ATOM	2113	CA	VAL	1706	29.560	14.576	7.474	1.00	31.80
ATOM	2114	CB	VAL	1706	28.483	15.632	7.172	1.00	34.66
ATOM	2115	CG1	VAL	1706	28.022	15.538	5.738	1.00	39.06
ATOM	2116	CG2	VAL	1706	27.309	15.455	8.106	1.00	36.62
ATOM	2117	C	VAL	1706	30.578	14.560	6.320	1.00	31.58
ATOM	2118	O	VAL	1706	30.682	13.585	5.570	1.00	32.35
ATOM	2119	N	GLU	1707	31.326	15.649	6.189	1.00	31.46
ATOM	2121	CA	GLU	1707	32.329	15.788	5.139	1.00	31.68
ATOM	2122	CB	GLU	1707	33.021	17.148	5.267	1.00	32.59
ATOM	2123	C	GLU	1707	33.381	14.678	5.114	1.00	32.23
ATOM	2124	O	GLU	1707	33.740	14.183	4.050	1.00	33.47
ATOM	2125	N	GLU	1708	33.902	14.316	6.279	1.00	32.90
ATOM	2127	CA	GLU	1708	34.909	13.268	6.352	1.00	33.86
ATOM	2128	CB	GLU	1708	35.570	13.244	7.730	1.00	38.54
ATOM	2129	CG	GLU	1708	36.190	14.575	8.165	1.00	47.63
ATOM	2130	CD	GLU	1708	37.442	14.962	7.383	1.00	58.35
ATOM	2131	OE1	GLU	1708	38.117	14.067	6.816	1.00	62.88
ATOM	2132	OE2	GLU	1708	37.770	16.176	7.355	1.00	64.79
ATOM	2133	C	GLU	1708	34.276	11.921	6.043	1.00	33.56
ATOM	2134	O	GLU	1708	34.927	11.038	5.489	1.00	34.18
ATOM	2135	N	LEU	1709	32.997	11.774	6.374	1.00	32.91
ATOM	2137	CA	LEU	1709	32.285	10.532	6.108	1.00	33.83
ATOM	2138	CB	LEU	1709	30.862	10.563	6.685	1.00	32.28
ATOM	2139	CG	LEU	1709	30.015	9.363	6.231	1.00	32.92
ATOM	2140	CD1	LEU	1709	30.541	8.071	6.853	1.00	28.37
ATOM	2141	CD2	LEU	1709	28.563	9.580	6.568	1.00	31.90
ATOM	2142	C	LEU	1709	32.222	10.283	4.606	1.00	34.15
ATOM	2143	O	LEU	1709	32.412	9.152	4.156	1.00	34.75
ATOM	2144	N	PHE	1710	31.918	11.332	3.844	1.00	33.83
ATOM	2146	CA	PHE	1710	31.828	11.248	2.388	1.00	32.90
ATOM	2147	CB	PHE	1710	31.531	12.622	1.787	1.00	34.85
ATOM	2148	CG	PHE	1710	30.162	13.132	2.082	1.00	38.60
ATOM	2149	CD1	PHE	1710	29.150	12.268	2.469	1.00	43.69
ATOM	2150	CD2	PHE	1710	29.882	14.480	1.984	1.00	45.10
ATOM	2151	CE1	PHE	1710	27.873	12.742	2.764	1.00	46.23
ATOM	2152	CE2	PHE	1710	28.611	14.966	2.274	1.00	48.15
ATOM	2153	CZ	PHE	1710	27.603	14.086	2.670	1.00	46.90
ATOM	2154	C	PHE	1710	33.131	10.739	1.803	1.00	31.84
ATOM	2155	O	PHE	1710	33.134	9.931	0.877	1.00	29.97
ATOM	2156	N	LYS	1711	34.231	11.224	2.373	1.00	32.45
ATOM	2158	CA	LYS	1711	35.582	10.860	1.947	1.00	34.53
ATOM	2159	CB	LYS	1711	36.588	11.755	2.675	1.00	36.17
ATOM	2160	CG	LYS	1711	38.008	11.669	2.182	1.00	41.07
ATOM	2161	CD	LYS	1711	38.912	12.582	3.001	1.00	46.23
ATOM	2162	CE	LYS	1711	40.311	12.648	2.418	1.00	51.79
ATOM	2163	NZ	LYS	1711	41.036	11.360	2.556	1.00	57.27
ATOM	2167	C	LYS	1711	35.867	9.375	2.215	1.00	33.82

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ATOM	2168	O	LYS	1711	36.451	8.688	1.376	1.00	33.20
ATOM	2169	N	LEU	1712	35.439	8.885	3.382	1.00	34.52
ATOM	2171	CA	LEU	1712	35.618	7.477	3.754	1.00	33.25
ATOM	2172	CB	LEU	1712	35.094	7.211	5.189	1.00	30.99
ATOM	2173	CG	LEU	1712	35.746	7.917	6.393	1.00	29.71
ATOM	2174	CD1	LEU	1712	35.047	7.552	7.678	1.00	24.11
ATOM	2175	CD2	LEU	1712	37.208	7.552	6.497	1.00	32.21
ATOM	2176	C	LEU	1712	34.833	6.631	2.744	1.00	32.16
ATOM	2177	O	LEU	1712	35.378	5.732	2.109	1.00	32.77
ATOM	2178	N	LEU	1713	33.562	6.967	2.563	1.00	31.72
ATOM	2180	CA	LEU	1713	32.700	6.259	1.637	1.00	33.60
ATOM	2181	CB	LEU	1713	31.299	6.879	1.619	1.00	36.57
ATOM	2182	CG	LEU	1713	30.522	6.711	2.930	1.00	37.60
ATOM	2183	CD1	LEU	1713	29.284	7.575	2.927	1.00	35.03
ATOM	2184	CD2	LEU	1713	30.182	5.246	3.157	1.00	33.22
ATOM	2185	C	LEU	1713	33.285	6.248	0.236	1.00	35.33
ATOM	2186	O	LEU	1713	33.318	5.203	-0.407	1.00	36.00
ATOM	2187	N	LYS	1714	33.741	7.405	-0.234	1.00	36.24
ATOM	2189	CA	LYS	1714	34.331	7.501	-1.566	1.00	36.35
ATOM	2190	CB	LYS	1714	34.707	8.946	-1.900	1.00	35.82
ATOM	2191	CG	LYS	1714	33.520	9.837	-2.168	1.00	37.23
ATOM	2192	CD	LYS	1714	32.712	9.324	-3.337	1.00	40.53
ATOM	2193	CE	LYS	1714	31.506	10.198	-3.600	1.00	44.51
ATOM	2194	NZ	LYS	1714	30.747	9.724	-4.804	1.00	50.76
ATOM	2198	C	LYS	1714	35.559	6.613	-1.701	1.00	37.60
ATOM	2199	O	LYS	1714	35.808	6.039	-2.764	1.00	40.82
ATOM	2200	N	GLU	1715	36.299	6.452	-0.615	1.00	35.61
ATOM	2202	CA	GLU	1715	37.496	5.630	-0.658	1.00	34.65
ATOM	2203	CB	GLU	1715	38.517	6.188	0.320	1.00	37.83
ATOM	2204	CG	GLU	1715	38.897	7.613	-0.036	1.00	42.28
ATOM	2205	CD	GLU	1715	39.634	8.342	1.061	1.00	45.64
ATOM	2206	OE1	GLU	1715	39.928	7.726	2.114	1.00	43.09
ATOM	2207	OE2	GLU	1715	39.918	9.544	0.853	1.00	47.56
ATOM	2208	C	GLU	1715	37.244	4.145	-0.419	1.00	32.94
ATOM	2209	O	GLU	1715	38.177	3.348	-0.419	1.00	33.31
ATOM	2210	N	GLY	1716	35.983	3.779	-0.213	1.00	29.12
ATOM	2212	CA	GLY	1716	35.634	2.391	0.004	1.00	26.02
ATOM	2213	C	GLY	1716	35.946	1.895	1.396	1.00	29.60
ATOM	2214	O	GLY	1716	36.223	0.715	1.588	1.00	29.81
ATOM	2215	N	HIS	1717	35.879	2.783	2.379	1.00	29.97
ATOM	2217	CA	HIS	1717	36.158	2.409	3.763	1.00	30.78
ATOM	2218	CB	HIS	1717	36.369	3.659	4.623	1.00	33.25
ATOM	2219	CG	HIS	1717	36.653	3.360	6.067	1.00	34.70
ATOM	2220	CD2	HIS	1717	37.820	3.155	6.715	1.00	32.77
ATOM	2221	ND1	HIS	1717	35.656	3.219	7.010	1.00	36.90
ATOM	2223	CE1	HIS	1717	36.200	2.932	8.180	1.00	35.87
ATOM	2224	NE2	HIS	1717	37.513	2.887	8.027	1.00	31.93
ATOM	2226	C	HIS	1717	35.035	1.577	4.375	1.00	29.63
ATOM	2227	O	HIS	1717	33.861	1.847	4.133	1.00	30.82
ATOM	2228	N	ARG	1718	35.406	0.600	5.201	1.00	27.92
ATOM	2230	CA	ARG	1718	34.436	-0.258	5.878	1.00	27.30
ATOM	2231	CB	ARG	1718	34.379	-1.641	5.236	1.00	24.10
ATOM	2232	CG	ARG	1718	33.939	-1.655	3.789	1.00	26.52
ATOM	2233	CD	ARG	1718	32.469	-1.288	3.627	1.00	26.96

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ATOM	2234	NE	ARG	1718	32.020	-1.374	2.232	1.00	24.41
ATOM	2236	CZ	ARG	1718	32.090	-0.377	1.352	1.00	25.51
ATOM	2237	NH1	ARG	1718	32.611	0.801	1.706	1.00	23.61
ATOM	2240	NH2	ARG	1718	31.553	-0.521	0.149	1.00	21.28
ATOM	2243	C	ARG	1718	34.881	-0.384	7.330	1.00	28.81
ATOM	2244	O	ARG	1718	36.080	-0.425	7.611	1.00	29.77
ATOM	2245	N	MET	1719	33.920	-0.377	8.250	1.00	30.40
ATOM	2247	CA	MET	1719	34.215	-0.485	9.673	1.00	30.62
ATOM	2248	CB	MET	1719	32.942	-0.339	10.497	1.00	28.91
ATOM	2249	CG	MET	1719	32.235	1.003	10.316	1.00	30.85
ATOM	2250	SD	MET	1719	30.829	1.237	11.432	1.00	33.27
ATOM	2251	CE	MET	1719	29.521	0.416	10.561	1.00	31.81
ATOM	2252	C	MET	1719	34.900	-1.793	10.005	1.00	31.32
ATOM	2253	O	MET	1719	34.755	-2.769	9.278	1.00	31.47
ATOM	2254	N	ASP	1720	35.651	-1.799	11.103	1.00	33.78
ATOM	2256	CA	ASP	1720	36.387	-2.983	11.550	1.00	33.45
ATOM	2257	CB	ASP	1720	37.478	-2.580	12.546	1.00	36.99
ATOM	2258	CG	ASP	1720	38.585	-1.762	11.908	1.00	41.56
ATOM	2259	OD1	ASP	1720	38.403	-1.339	10.742	1.00	48.43
ATOM	2260	OD2	ASP	1720	39.634	-1.546	12.568	1.00	40.99
ATOM	2261	C	ASP	1720	35.473	-4.001	12.211	1.00	32.12
ATOM	2262	O	ASP	1720	34.381	-3.657	12.668	1.00	30.89
ATOM	2263	N	LYS	1721	35.944	-5.241	12.328	1.00	31.82
ATOM	2265	CA	LYS	1721	35.127	-6.270	12.953	1.00	31.71
ATOM	2266	CB	LYS	1721	35.691	-7.679	12.747	1.00	32.34
ATOM	2267	CG	LYS	1721	34.762	-8.738	13.344	1.00	34.85
ATOM	2268	CD	LYS	1721	35.111	-10.155	12.961	1.00	37.39
ATOM	2269	CE	LYS	1721	35.266	-10.674	13.765	1.00	41.42
ATOM	2270	NZ	LYS	1721	36.348	-12.154	13.635	1.00	46.55
ATOM	2274	C	LYS	1721	35.007	-6.018	14.430	1.00	33.40
ATOM	2275	O	LYS	1721	36.017	-5.879	15.121	1.00	34.26
ATOM	2276	N	PRO	1722	33.768	-5.924	14.934	1.00	34.26
ATOM	2277	CD	PRO	1722	32.494	-6.002	14.203	1.00	32.16
ATOM	2278	CA	PRO	1722	33.546	-5.692	16.362	1.00	35.84
ATOM	2279	CB	PRO	1722	32.027	-5.682	16.473	1.00	35.35
ATOM	2280	CG	PRO	1722	31.575	-5.255	15.108	1.00	35.35
ATOM	2281	C	PRO	1722	34.105	-6.904	17.099	1.00	40.41
ATOM	2282	O	PRO	1722	34.010	-8.038	16.607	1.00	41.14
ATOM	2283	N	SER	1723	34.739	-6.680	18.240	1.00	43.60
ATOM	2285	CA	SER	1723	35.260	-7.808	18.999	1.00	45.51
ATOM	2286	CB	SER	1723	36.078	-7.324	20.191	1.00	45.30
ATOM	2287	OG	SER	1723	35.384	-6.300	20.879	1.00	49.62
ATOM	2289	C	SER	1723	34.031	-8.589	19.460	1.00	46.39
ATOM	2290	O	SER	1723	32.939	-8.028	19.614	1.00	45.16
ATOM	2291	N	ASN	1724	34.199	-9.891	19.631	1.00	48.53
ATOM	2293	CA	ASN	1724	33.088	-10.723	20.065	1.00	51.13
ATOM	2294	CB	ASN	1724	32.509	-10.194	21.390	1.00	56.87
ATOM	2295	CG	ASN	1724	33.595	-9.892	22.427	1.00	61.65
ATOM	2296	OD1	ASN	1724	34.503	-10.702	22.649	1.00	63.73
ATOM	2297	ND2	ASN	1724	33.526	-8.713	23.039	1.00	64.64
ATOM	2300	C	ASN	1724	32.034	-10.743	18.941	1.00	48.83
ATOM	2301	O	ASN	1724	30.846	-10.534	19.145	1.00	50.50
ATOM	2302	N	CYS	1725	32.511	-10.977	17.734	1.00	45.23
ATOM	2304	CA	CYS	1725	31.654	-11.056	16.570	1.00	42.33

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ATOM	2305	CB	CYS	1725	31.570	-9.702	15.854	1.00	41.48
ATOM	2306	SG	CYS	1725	30.711	-9.751	14.275	1.00	40.38
ATOM	2307	C	CYS	1725	32.383	-12.077	15.725	1.00	39.64
ATOM	2308	O	CYS	1725	33.601	-12.004	15.579	1.00	42.00
ATOM	2309	N	THR	1726	31.664	-13.090	15.263	1.00	35.96
ATOM	2311	CA	THR	1726	32.275	-14.139	14.459	1.00	33.61
ATOM	2312	CB	THR	1726	31.301	-15.326	14.326	1.00	33.29
ATOM	2313	OG1	THR	1726	30.071	-14.904	13.711	1.00	34.53
ATOM	2315	CG2	THR	1726	30.981	-15.861	15.696	1.00	25.84
ATOM	2316	C	THR	1726	32.720	-13.629	13.092	1.00	32.27
ATOM	2317	O	THR	1726	32.257	-12.593	12.643	1.00	33.04
ATOM	2318	N	ASN	1727	33.643	-14.315	12.434	1.00	32.98
ATOM	2320	CA	ASN	1727	34.050	-13.850	11.114	1.00	34.97
ATOM	2321	CB	ASN	1727	35.198	-14.680	10.541	1.00	39.89
ATOM	2322	CG	ASN	1727	36.540	-14.271	11.103	1.00	45.37
ATOM	2323	OD1	ASN	1727	37.044	-13.177	10.826	1.00	48.43
ATOM	2324	ND2	ASN	1727	37.125	-15.141	11.909	1.00	45.88
ATOM	2327	C	ASN	1727	32.846	-13.947	10.192	1.00	33.97
ATOM	2328	O	ASN	1727	32.646	-13.088	9.341	1.00	35.07
ATOM	2329	N	GLU	1728	32.024	-14.973	10.414	1.00	31.69
ATOM	2331	CA	GLU	1728	30.814	-15.210	9.620	1.00	30.27
ATOM	2332	CB	GLU	1728	30.141	-16.493	10.083	1.00	32.53
ATOM	2333	CG	GLU	1728	28.932	-16.878	9.273	1.00	32.81
ATOM	2334	CD	GLU	1728	28.353	-18.190	9.711	1.00	36.43
ATOM	2335	OE1	GLU	1728	28.339	-18.466	10.932	1.00	36.75
ATOM	2336	OE2	GLU	1728	27.908	-18.945	8.829	1.00	41.92
ATOM	2337	C	GLU	1728	29.814	-14.049	9.681	1.00	28.70
ATOM	2338	O	GLU	1728	29.234	-13.655	8.660	1.00	28.51
ATOM	2339	N	LEU	1729	29.594	-13.517	10.880	1.00	26.77
ATOM	2341	CA	LEU	1729	28.687	-12.393	11.040	1.00	26.80
ATOM	2342	CB	LEU	1729	28.228	-12.274	12.490	1.00	27.91
ATOM	2343	CG	LEU	1729	27.233	-13.355	12.913	1.00	30.71
ATOM	2344	CD1	LEU	1729	27.095	-13.345	14.428	1.00	35.79
ATOM	2345	CD2	LEU	1729	25.885	-13.141	12.253	1.00	25.70
ATOM	2346	C	LEU	1729	29.319	-11.089	10.540	1.00	27.06
ATOM	2347	O	LEU	1729	28.610	-10.177	10.126	1.00	30.27
ATOM	2348	N	TYR	1730	30.650	-11.004	10.549	1.00	27.03
ATOM	2350	CA	TYR	1730	31.328	-9.812	10.039	1.00	26.21
ATOM	2351	CB	TYR	1730	32.792	-9.778	10.474	1.00	25.31
ATOM	2352	CG	TYR	1730	33.538	-8.553	9.982	1.00	24.89
ATOM	2353	CD1	TYR	1730	33.012	-7.270	10.169	1.00	23.59
ATOM	2354	CE1	TYR	1730	33.655	-6.148	9.665	1.00	24.74
ATOM	2355	CD2	TYR	1730	34.739	-8.675	9.285	1.00	22.11
ATOM	2356	CE2	TYR	1730	35.399	-7.560	8.775	1.00	22.32
ATOM	2357	CZ	TYR	1730	34.853	-6.295	8.962	1.00	26.07
ATOM	2358	OH	TYR	1730	35.484	-5.181	8.418	1.00	22.70
ATOM	2360	C	TYR	1730	31.227	-9.878	8.509	1.00	27.71
ATOM	2361	O	TYR	1730	30.960	-8.875	7.843	1.00	28.05
ATOM	2362	N	MET	1731	31.409	-11.081	7.977	1.00	27.92
ATOM	2364	CA	MET	1731	31.306	-11.355	6.548	1.00	28.89
ATOM	2365	CB	MET	1731	31.506	-12.853	6.317	1.00	35.84
ATOM	2366	CG	MET	1731	31.068	-13.379	4.975	1.00	45.50
ATOM	2367	SD	MET	1731	31.347	-15.167	4.865	1.00	56.40
ATOM	2368	CE	MET	1731	32.106	-15.263	3.217	1.00	56.88

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ATOM	2369	C	MET	1731	29.916	-10.928	6.102	1.00	27.79
ATOM	2370	O	MET	1731	29.755	-10.345	5.041	1.00	30.68
ATOM	2371	N	MET	1732	28.915	-11.203	6.932	1.00	28.02
ATOM	2373	CA	MET	1732	27.546	-10.804	6.639	1.00	25.74
ATOM	2374	CB	MET	1732	26.598	-11.317	7.718	1.00	24.94
ATOM	2375	CG	MET	1732	25.153	-10.911	7.492	1.00	22.96
ATOM	2376	SD	MET	1732	24.008	-11.593	8.684	1.00	24.39
ATOM	2377	CE	MET	1732	23.798	-13.272	8.002	1.00	18.04
ATOM	2378	C	MET	1732	27.470	-9.273	6.559	1.00	25.81
ATOM	2379	O	MET	1732	26.889	-8.729	5.620	1.00	26.85
ATOM	2380	N	MET	1733	28.068	-8.587	7.537	1.00	24.84
ATOM	2382	CA	MET	1733	28.092	-7.124	7.545	1.00	25.27
ATOM	2383	CB	MET	1733	28.931	-6.600	8.700	1.00	25.97
ATOM	2384	CG	MET	1733	28.342	-6.769	10.058	1.00	28.69
ATOM	2385	SD	MET	1733	29.456	-6.094	11.295	1.00	29.06
ATOM	2386	CE	MET	1733	28.927	-7.051	12.693	1.00	28.07
ATOM	2387	C	MET	1733	28.741	-6.628	6.270	1.00	26.97
ATOM	2388	O	MET	1733	28.192	-5.771	5.581	1.00	28.37
ATOM	2389	N	ARG	1734	29.922	-7.160	5.966	1.00	28.77
ATOM	2391	CA	ARG	1734	30.664	-6.775	4.762	1.00	29.66
ATOM	2392	CB	ARG	1734	32.027	-7.482	4.716	1.00	29.05
ATOM	2393	CG	ARG	1734	32.968	-7.109	5.866	1.00	25.00
ATOM	2394	CD	ARG	1734	33.247	-5.621	5.882	1.00	29.27
ATOM	2395	NE	ARG	1734	33.911	-5.210	4.647	1.00	35.43
ATOM	2397	CZ	ARG	1734	35.233	-5.220	4.466	1.00	38.24
ATOM	2398	NH1	ARG	1734	36.054	-5.601	5.445	1.00	36.47
ATOM	2401	NH2	ARG	1734	35.732	-4.907	3.277	1.00	38.57
ATOM	2404	C	ARG	1734	29.859	-7.034	3.478	1.00	29.57
ATOM	2405	O	ARG	1734	29.920	-6.242	2.538	1.00	29.55
ATOM	2406	N	ASP	1735	29.095	-8.124	3.448	1.00	28.07
ATOM	2408	CA	ASP	1735	28.259	-8.423	2.287	1.00	27.96
ATOM	2409	CB	ASP	1735	27.634	-9.813	2.408	1.00	28.60
ATOM	2410	CG	ASP	1735	28.664	-10.926	2.283	1.00	31.34
ATOM	2411	OD1	ASP	1735	29.785	-10.660	1.798	1.00	31.12
ATOM	2412	OD2	ASP	1735	28.356	-12.068	2.687	1.00	36.07
ATOM	2413	C	ASP	1735	27.159	-7.368	2.155	1.00	27.24
ATOM	2414	O	ASP	1735	26.846	-6.932	1.050	1.00	25.79
ATOM	2415	N	CYS	1736	26.590	-6.951	3.288	1.00	26.53
ATOM	2417	CA	CYS	1736	25.547	-5.930	3.314	1.00	24.35
ATOM	2418	CB	CYS	1736	24.968	-5.765	4.731	1.00	22.01
ATOM	2419	SG	CYS	1736	23.885	-7.101	5.281	1.00	21.52
ATOM	2420	C	CYS	1736	26.119	-4.595	2.847	1.00	24.26
ATOM	2421	O	CYS	1736	25.386	-3.725	2.368	1.00	24.19
ATOM	2422	N	TRP	1737	27.432	-4.437	3.002	1.00	22.94
ATOM	2424	CA	TRP	1737	28.104	-3.210	2.605	1.00	21.91
ATOM	2425	CB	TRP	1737	29.146	-2.820	3.640	1.00	19.26
ATOM	2426	CG	TRP	1737	28.572	-2.493	4.947	1.00	20.89
ATOM	2427	CD2	TRP	1737	29.226	-2.602	6.212	1.00	23.33
ATOM	2428	CE2	TRP	1737	28.315	-2.159	7.196	1.00	21.59
ATOM	2429	CE3	TRP	1737	30.506	-3.026	6.614	1.00	25.00
ATOM	2430	CD1	TRP	1737	27.319	-2.012	5.201	1.00	19.90
ATOM	2431	NE1	TRP	1737	27.158	-1.807	6.551	1.00	20.77
ATOM	2433	CZ2	TRP	1737	28.641	-2.127	8.563	1.00	19.89
ATOM	2434	CZ3	TRP	1737	30.825	-2.993	7.971	1.00	21.23

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ATOM	2435	CH2	TRP	1737	29.896	-2.543	8.927	1.00	21.09
ATOM	2436	C	TRP	1737	28.758	-3.266	1.232	1.00	23.54
ATOM	2437	O	TRP	1737	29.653	-2.477	0.939	1.00	24.68
ATOM	2438	N	HIS	1738	28.315	-4.185	0.382	1.00	24.37
ATOM	2440	CA	HIS	1738	28.877	-4.287	-0.947	1.00	24.42
ATOM	2441	CB	HIS	1738	28.243	-5.436	-1.728	1.00	23.72
ATOM	2442	CG	HIS	1738	29.131	-5.985	-2.801	1.00	27.20
ATOM	2443	CD2	HIS	1738	29.595	-5.425	-3.948	1.00	26.45
ATOM	2444	ND1	HIS	1738	29.681	-7.255	-2.751	1.00	29.26
ATOM	2446	CE1	HIS	1738	30.436	-7.441	-3.816	1.00	29.25
ATOM	2447	NE2	HIS	1738	30.409	-6.358	-4.556	1.00	27.32
ATOM	2449	C	HIS	1738	28.716	-2.970	-1.713	1.00	25.82
ATOM	2450	O	HIS	1738	27.675	-2.314	-1.660	1.00	23.96
ATOM	2451	N	ALA	1739	29.802	-2.564	-2.362	1.00	26.27
ATOM	2453	CA	ALA	1739	29.825	-1.346	-3.158	1.00	25.46
ATOM	2454	CB	ALA	1739	31.186	-1.180	-3.789	1.00	25.70
ATOM	2455	C	ALA	1739	28.754	-1.443	-4.233	1.00	26.18
ATOM	2456	O	ALA	1739	28.116	-0.455	-4.574	1.00	29.14
ATOM	2457	N	VAL	1740	28.570	-2.643	-4.774	1.00	25.71
ATOM	2459	CA	VAL	1740	27.560	-2.875	-5.802	1.00	26.12
ATOM	2460	CB	VAL	1740	28.063	-3.841	-6.903	1.00	25.99
ATOM	2461	CG1	VAL	1740	27.102	-3.832	-8.090	1.00	23.37
ATOM	2462	CG2	VAL	1740	29.450	-3.440	-7.349	1.00	22.07
ATOM	2463	C	VAL	1740	26.247	-3.400	-5.191	1.00	25.43
ATOM	2464	O	VAL	1740	26.186	-4.550	-4.704	1.00	24.93
ATOM	2465	N	PRO	1741	25.170	-2.585	-5.265	1.00	24.20
ATOM	2466	CD	PRO	1741	25.151	-1.277	-5.953	1.00	18.88
ATOM	2467	CA	PRO	1741	23.838	-2.914	-4.734	1.00	25.28
ATOM	2468	CB	PRO	1741	22.953	-1.788	-5.294	1.00	22.75
ATOM	2469	CG	PRO	1741	23.903	-0.632	-5.398	1.00	20.99
ATOM	2470	C	PRO	1741	23.299	-4.296	-5.128	1.00	25.84
ATOM	2471	O	PRO	1741	22.787	-5.036	-4.280	1.00	25.99
ATOM	2472	N	SER	1742	23.425	-4.642	-6.407	1.00	26.48
ATOM	2474	CA	SER	1742	22.942	-5.919	-6.930	1.00	25.19
ATOM	2475	CB	SER	1742	23.151	-5.992	-8.440	1.00	25.68
ATOM	2476	OG	SER	1742	24.530	-5.943	-8.769	1.00	27.46
ATOM	2478	C	SER	1742	23.644	-7.100	-6.289	1.00	25.24
ATOM	2479	O	SER	1742	23.124	-8.218	-6.300	1.00	26.09
ATOM	2480	N	GLN	1743	24.826	-6.851	-5.731	1.00	23.88
ATOM	2482	CA	GLN	1743	25.590	-7.917	-5.118	1.00	24.44
ATOM	2483	CB	GLN	1743	27.069	-7.733	-5.437	1.00	27.26
ATOM	2484	CG	GLN	1743	27.344	-7.784	-6.940	1.00	27.39
ATOM	2485	CD	GLN	1743	26.803	-9.047	-7.581	1.00	26.46
ATOM	2486	OE1	GLN	1743	27.325	-10.136	-7.339	1.00	25.80
ATOM	2487	NE2	GLN	1743	25.760	-8.914	-8.393	1.00	27.42
ATOM	2490	C	GLN	1743	25.348	-8.151	-3.633	1.00	23.20
ATOM	2491	O	GLN	1743	25.810	-9.147	-3.083	1.00	22.90
ATOM	2492	N	ARG	1744	24.628	-7.243	-2.984	1.00	22.15
ATOM	2494	CA	ARG	1744	24.318	-7.398	-1.568	1.00	21.23
ATOM	2495	CB	ARG	1744	23.767	-6.088	-0.998	1.00	19.01
ATOM	2496	CG	ARG	1744	24.705	-4.916	-1.145	1.00	17.27
ATOM	2497	CD	ARG	1744	24.091	-3.605	-0.679	1.00	14.79
ATOM	2498	NE	ARG	1744	24.914	-2.493	-1.157	1.00	19.72
ATOM	2500	CZ	ARG	1744	24.482	-1.258	-1.391	1.00	19.23

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ATOM	2501	NH1	ARG	1744	23.201	-0.931	-1.201	1.00	15.90
ATOM	2504	NH2	ARG	1744	25.343	-0.343	-1.821	1.00	19.43
ATOM	2507	C	ARG	1744	23.259	-8.496	-1.438	1.00	21.95
ATOM	2508	O	ARG	1744	22.585	-8.827	-2.415	1.00	25.34
ATOM	2509	N	PRO	1745	23.213	-9.184	-0.292	1.00	20.82
ATOM	2510	CD	PRO	1745	24.191	-9.219	0.804	1.00	21.25
ATOM	2511	CA	PRO	1745	22.204	-10.229	-0.127	1.00	21.39
ATOM	2512	CB	PRO	1745	22.687	-10.980	1.117	1.00	21.69
ATOM	2513	CG	PRO	1745	23.418	-9.916	1.886	1.00	22.62
ATOM	2514	C	PRO	1745	20.833	-9.585	0.102	1.00	22.15
ATOM	2515	O	PRO	1745	20.739	-8.402	0.426	1.00	23.29
ATOM	2516	N	THR	1746	19.771	-10.349	-0.109	1.00	20.93
ATOM	2518	CA	THR	1746	18.440	-9.827	0.107	1.00	19.90
ATOM	2519	CB	THR	1746	17.391	-10.554	-0.783	1.00	20.21
ATOM	2520	OG1	THR	1746	17.484	-11.974	-0.584	1.00	22.03
ATOM	2522	CG2	THR	1746	17.609	-10.242	-2.255	1.00	20.82
ATOM	2523	C	THR	1746	18.112	-10.095	1.557	1.00	19.77
ATOM	2524	O	THR	1746	18.842	-10.823	2.228	1.00	19.19
ATOM	2525	N	PHE	1747	17.010	-9.526	2.045	1.00	23.46
ATOM	2527	CA	PHE	1747	16.582	-9.770	3.422	1.00	21.64
ATOM	2528	CB	PHE	1747	15.473	-8.794	3.827	1.00	18.89
ATOM	2529	CG	PHE	1747	15.987	-7.445	4.262	1.00	17.45
ATOM	2530	CD1	PHE	1747	16.757	-7.317	5.417	1.00	17.65
ATOM	2531	CD2	PHE	1747	15.712	-6.303	3.516	1.00	15.37
ATOM	2532	CE1	PHE	1747	17.242	-6.073	5.819	1.00	16.17
ATOM	2533	CE2	PHE	1747	16.189	-5.056	3.907	1.00	14.53
ATOM	2534	CZ	PHE	1747	16.959	-4.941	5.065	1.00	16.88
ATOM	2535	C	PHE	1747	16.118	-11.227	3.522	1.00	23.18
ATOM	2536	O	PHE	1747	16.271	-11.873	4.548	1.00	24.04
ATOM	2537	N	LYS	1748	15.570	-11.745	2.432	1.00	24.13
ATOM	2539	CA	LYS	1748	15.137	-13.132	2.385	1.00	26.35
ATOM	2540	CB	LYS	1748	14.502	-13.424	1.024	1.00	27.52
ATOM	2541	CG	LYS	1748	14.034	-14.849	0.836	1.00	33.88
ATOM	2542	CD	LYS	1748	13.598	-15.062	-0.600	1.00	41.83
ATOM	2543	CE	LYS	1748	13.190	-16.506	-0.881	1.00	50.05
ATOM	2544	NZ	LYS	1748	12.084	-16.986	0.005	1.00	55.70
ATOM	2548	C	LYS	1748	16.359	-14.037	2.636	1.00	27.50
ATOM	2549	O	LYS	1748	16.303	-14.950	3.459	1.00	31.18
ATOM	2550	N	GLN	1749	17.467	-13.761	1.949	1.00	27.24
ATOM	2552	CA	GLN	1749	18.699	-14.529	2.122	1.00	27.03
ATOM	2553	CB	GLN	1749	19.797	-14.039	1.169	1.00	31.80
ATOM	2554	CG	GLN	1749	19.501	-14.196	-0.323	1.00	38.57
ATOM	2555	CD	GLN	1749	20.460	-13.385	-1.209	1.00	39.93
ATOM	2556	OE1	GLN	1749	20.025	-12.535	-1.974	1.00	39.90
ATOM	2557	NE2	GLN	1749	21.768	-13.620	-1.068	1.00	40.23
ATOM	2560	C	GLN	1749	19.205	-14.380	3.552	1.00	25.98
ATOM	2561	O	GLN	1749	19.533	-15.371	4.198	1.00	27.18
ATOM	2562	N	LEU	1750	19.293	-13.133	4.018	1.00	25.20
ATOM	2564	CA	LEU	1750	19.774	-12.823	5.369	1.00	25.74
ATOM	2565	CB	LEU	1750	19.722	-11.317	5.631	1.00	20.99
ATOM	2566	CG	LEU	1750	20.708	-10.468	4.831	1.00	20.90
ATOM	2567	CD1	LEU	1750	20.302	-8.987	4.822	1.00	19.88
ATOM	2568	CD2	LEU	1750	22.071	-10.643	5.426	1.00	17.26
ATOM	2569	C	LEU	1750	18.985	-13.555	6.441	1.00	27.10

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ATOM	2570	O	LEU	1750	19.553	-14.094	7.392	1.00	27.89
ATOM	2571	N	VAL	1751	17.672	-13.598	6.265	1.00	29.40
ATOM	2573	CA	VAL	1751	16.798	-14.262	7.210	1.00	26.80
ATOM	2574	CB	VAL	1751	15.324	-14.030	6.843	1.00	26.94
ATOM	2575	CG1	VAL	1751	14.429	-14.941	7.657	1.00	29.93
ATOM	2576	CG2	VAL	1751	14.941	-12.575	7.117	1.00	24.10
ATOM	2577	C	VAL	1751	17.136	-15.745	7.228	1.00	27.80
ATOM	2578	O	VAL	1751	17.223	-16.359	8.285	1.00	26.77
ATOM	2579	N	GLU	1752	17.408	-16.300	6.056	1.00	32.26
ATOM	2581	CA	GLU	1752	17.749	-17.717	5.966	1.00	35.72
ATOM	2582	CB	GLU	1752	17.721	-18.173	4.504	1.00	39.33
ATOM	2583	CG	GLU	1752	16.306	-18.078	3.911	1.00	49.41
ATOM	2584	CD	GLU	1752	16.209	-18.421	2.429	1.00	55.88
ATOM	2585	OE1	GLU	1752	15.141	-18.138	1.835	1.00	58.00
ATOM	2586	OE2	GLU	1752	17.180	-18.978	1.863	1.00	61.03
ATOM	2587	C	GLU	1752	19.093	-18.002	6.635	1.00	34.59
ATOM	2588	O	GLU	1752	19.230	-18.975	7.393	1.00	33.95
ATOM	2589	N	ASP	1753	20.057	-17.114	6.401	1.00	34.38
ATOM	2591	CA	ASP	1753	21.393	-17.235	6.977	1.00	32.81
ATOM	2592	CB	ASP	1753	22.338	-16.227	6.334	1.00	31.57
ATOM	2593	CG	ASP	1753	22.628	-16.556	4.888	1.00	33.68
ATOM	2594	OD1	ASP	1753	22.573	-17.755	4.536	1.00	35.14
ATOM	2595	OD2	ASP	1753	22.914	-15.624	4.104	1.00	34.44
ATOM	2596	C	ASP	1753	21.378	-17.058	8.489	1.00	32.04
ATOM	2597	O	ASP	1753	21.997	-17.837	9.214	1.00	31.21
ATOM	2598	N	LEU	1754	20.648	-16.045	8.955	1.00	31.00
ATOM	2600	CA	LEU	1754	20.528	-15.754	10.382	1.00	29.46
ATOM	2601	CB	LEU	1754	19.822	-14.426	10.598	1.00	23.47
ATOM	2602	CG	LEU	1754	20.816	-13.309	10.318	1.00	23.58
ATOM	2603	CD1	LEU	1754	20.114	-11.963	10.128	1.00	20.46
ATOM	2604	CD2	LEU	1754	21.828	-13.282	11.462	1.00	19.18
ATOM	2605	C	LEU	1754	19.806	-16.866	11.110	1.00	31.84
ATOM	2606	O	LEU	1754	20.125	-17.178	12.254	1.00	30.78
ATOM	2607	N	ASP	1755	18.832	-17.471	10.445	1.00	34.03
ATOM	2609	CA	ASP	1755	18.116	-18.578	11.044	1.00	35.22
ATOM	2610	CB	ASP	1755	16.973	-19.027	10.148	1.00	38.40
ATOM	2611	CG	ASP	1755	16.159	-20.119	10.779	1.00	41.85
ATOM	2612	OD1	ASP	1755	15.560	-19.866	11.841	1.00	47.90
ATOM	2613	OD2	ASP	1755	16.142	-21.241	10.238	1.00	46.67
ATOM	2614	C	ASP	1755	19.114	-19.724	11.222	1.00	36.79
ATOM	2615	O	ASP	1755	19.114	-20.411	12.250	1.00	38.33
ATOM	2616	N	ARG	1756	19.973	-19.920	10.226	1.00	34.81
ATOM	2618	CA	ARG	1756	20.982	-20.969	10.302	1.00	34.68
ATOM	2619	CB	ARG	1756	21.688	-21.100	8.959	1.00	34.78
ATOM	2620	CG	ARG	1756	22.746	-22.179	8.910	1.00	35.93
ATOM	2621	CD	ARG	1756	23.297	-22.306	7.511	1.00	41.60
ATOM	2622	NE	ARG	1756	23.786	-21.025	6.999	1.00	46.42
ATOM	2624	CZ	ARG	1756	24.889	-20.419	7.427	1.00	48.38
ATOM	2625	NH1	ARG	1756	25.637	-20.976	8.381	1.00	48.10
ATOM	2628	NH2	ARG	1756	25.236	-19.242	6.909	1.00	46.62
ATOM	2631	C	ARG	1756	22.002	-20.666	11.399	1.00	36.17
ATOM	2632	O	ARG	1756	22.372	-21.541	12.177	1.00	38.33
ATOM	2633	N	ILE	1757	22.433	-19.413	11.478	1.00	37.00
ATOM	2635	CA	ILE	1757	23.416	-18.998	12.468	1.00	35.60

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ATOM	2636	CB	ILE	1757	23.964	-17.588	12.141	1.00	35.54
ATOM	2637	CG2	ILE	1757	24.921	-17.131	13.217	1.00	32.41
ATOM	2638	CG1	ILE	1757	24.693	-17.612	10.794	1.00	33.77
ATOM	2639	CD1	ILE	1757	25.097	-16.253	10.287	1.00	33.49
ATOM	2640	C	ILE	1757	22.866	-19.048	13.891	1.00	37.28
ATOM	2641	O	ILE	1757	23.531	-19.556	14.779	1.00	38.42
ATOM	2642	N	VAL	1758	21.634	-18.585	14.088	1.00	39.19
ATOM	2644	CA	VAL	1758	21.016	-18.584	15.421	1.00	39.84
ATOM	2645	CB	VAL	1758	19.560	-18.017	15.403	1.00	37.62
ATOM	2646	CG1	VAL	1758	18.918	-18.144	16.773	1.00	38.30
ATOM	2647	CG2	VAL	1758	19.560	-16.560	15.009	1.00	39.62
ATOM	2648	C	VAL	1758	20.983	-19.997	15.988	1.00	41.98
ATOM	2649	O	VAL	1758	21.380	-20.229	17.128	1.00	43.36
ATOM	2650	N	ALA	1759	20.501	-20.932	15.182	1.00	43.31
ATOM	2652	CA	ALA	1759	20.418	-22.325	15.589	1.00	44.00
ATOM	2653	CB	ALA	1759	19.836	-23.150	14.459	1.00	44.52
ATOM	2654	C	ALA	1759	21.784	-22.867	15.976	1.00	45.98
ATOM	2655	O	ALA	1759	21.894	-23.725	16.841	1.00	48.78
ATOM	2656	N	LEU	1760	22.823	-22.375	15.319	1.00	48.93
ATOM	2658	CA	LEU	1760	24.175	-22.831	15.592	1.00	51.47
ATOM	2659	CB	LEU	1760	24.954	-22.900	14.280	1.00	53.63
ATOM	2660	CG	LEU	1760	24.284	-23.864	13.295	1.00	57.84
ATOM	2661	CD1	LEU	1760	24.993	-23.847	11.948	1.00	61.83
ATOM	2662	CD2	LEU	1760	24.260	-25.277	13.886	1.00	58.57
ATOM	2663	C	LEU	1760	24.911	-21.965	16.607	1.00	53.60
ATOM	2664	O	LEU	1760	26.078	-22.214	16.919	1.00	54.00
ATOM	2665	N	THR	1761	24.222	-20.963	17.141	1.00	55.77
ATOM	2667	CA	THR	1761	24.820	-20.060	18.111	1.00	56.64
ATOM	2668	CB	THR	1761	24.250	-18.627	17.979	1.00	55.76
ATOM	2669	OG1	THR	1761	24.444	-18.154	16.644	1.00	56.20
ATOM	2671	CG2	THR	1761	24.962	-17.680	18.917	1.00	55.25
ATOM	2672	C	THR	1761	24.636	-20.548	19.539	1.00	58.16
ATOM	2673	O	THR	1761	23.566	-21.021	19.919	1.00	56.85
ATOM	2674	N	SER	1762	25.706	-20.436	20.318	1.00	61.74
ATOM	2676	CA	SER	1762	25.706	-20.833	21.717	1.00	64.50
ATOM	2677	CB	SER	1762	27.155	-20.979	22.205	1.00	68.82
ATOM	2678	OG	SER	1762	27.232	-21.544	23.508	1.00	73.15
ATOM	2680	C	SER	1762	24.965	-19.775	22.547	1.00	63.87
ATOM	2681	O	SER	1762	25.080	-18.563	22.296	1.00	63.22
ATOM	3420	PA	PCP	400	62.748	10.301	7.817	1.00	90.90
ATOM	3421	O1A	PCP	400	62.509	10.036	9.280	1.00	92.35
ATOM	3422	O2A	PCP	400	61.832	11.180	7.038	1.00	90.49
ATOM	3423	O5*	PCP	400	62.744	8.904	7.142	1.00	83.57
ATOM	3424	PB	PCP	400	65.226	11.946	8.294	1.00	101.51
ATOM	3425	O1B	PCP	400	65.246	13.015	7.264	1.00	102.85
ATOM	3426	O2B	PCP	400	66.527	11.458	8.830	1.00	99.88
ATOM	3427	O3A	PCP	400	64.334	10.725	7.584	1.00	96.64
ATOM	3428	C3B	PCP	400	64.345	12.502	9.635	1.00	102.94
ATOM	3429	C5*	PCP	400	62.337	8.684	5.839	1.00	71.21
ATOM	3430	C4*	PCP	400	62.479	7.204	5.587	1.00	64.48
ATOM	3431	O4*	PCP	400	63.713	6.745	6.169	1.00	60.91
ATOM	3432	C1*	PCP	400	63.394	5.459	6.680	1.00	54.96
ATOM	3433	N9	PCP	400	64.326	5.101	7.712	1.00	47.26
ATOM	3434	C4	PCP	400	65.017	3.903	7.840	1.00	46.24

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ATOM	3435	N3	PCP	400	64.926	2.770	7.062	1.00	41.02
ATOM	3436	C2	PCP	400	65.802	1.878	7.531	1.00	40.72
ATOM	3437	N1	PCP	400	66.674	1.917	8.558	1.00	37.37
ATOM	3438	C6	PCP	400	66.735	3.028	9.305	1.00	40.23
ATOM	3439	N6	PCP	400	67.573	3.134	10.333	1.00	33.92
ATOM	3442	C5	PCP	400	65.862	4.091	8.937	1.00	44.12
ATOM	3443	N7	PCP	400	65.674	5.361	9.472	1.00	45.15
ATOM	3444	C8	PCP	400	64.761	5.894	8.702	1.00	44.83
ATOM	3445	C2*	PCP	400	61.986	5.500	7.254	1.00	57.63
ATOM	3446	O2*	PCP	400	61.454	4.153	7.211	1.00	56.45
ATOM	3448	C3*	PCP	400	61.328	6.402	6.245	1.00	61.31
ATOM	3449	O3*	PCP	400	60.689	5.644	5.206	1.00	64.65
ATOM	3451	PA	PCP	401	9.366	9.801	17.743	0.50	74.43
ATOM	3452	O1A	PCP	401	9.463	8.736	16.709	0.50	75.37
ATOM	3453	O2A	PCP	401	10.330	10.926	17.699	0.50	75.86
ATOM	3454	O5*	PCP	401	9.427	9.108	19.186	0.50	67.44
ATOM	3455	PB	PCP	401	6.878	10.679	16.547	0.50	82.27
ATOM	3456	O1B	PCP	401	6.223	11.982	16.778	0.50	82.91
ATOM	3457	O2B	PCP	401	6.020	9.486	16.408	0.50	82.70
ATOM	3458	O3A	PCP	401	7.868	10.423	17.814	0.50	78.30
ATOM	3459	C3B	PCP	401	7.790	10.845	15.159	0.50	82.50
ATOM	3460	C5*	PCP	401	10.184	9.593	20.275	0.50	54.44
ATOM	3461	C4*	PCP	401	10.228	8.637	21.442	0.50	45.38
ATOM	3462	O4*	PCP	401	9.032	7.855	21.412	0.50	39.40
ATOM	3463	C1*	PCP	401	9.397	6.509	21.641	0.50	35.00
ATOM	3464	N9	PCP	401	8.386	5.627	21.044	0.50	27.91
ATOM	3465	C4	PCP	401	7.790	4.469	21.564	0.50	23.36
ATOM	3466	N3	PCP	401	7.982	3.849	22.732	0.50	22.33
ATOM	3467	C2	PCP	401	7.239	2.768	22.838	0.50	20.26
ATOM	3468	N1	PCP	401	6.382	2.251	22.003	0.50	17.29
ATOM	3469	C6	PCP	401	6.202	2.877	20.856	0.50	19.35
ATOM	3470	N6	PCP	401	5.327	2.415	19.975	0.50	16.87
ATOM	3473	C5	PCP	401	6.932	4.038	20.603	0.50	21.72
ATOM	3474	N7	PCP	401	6.983	4.880	19.507	0.50	24.59
ATOM	3475	C8	PCP	401	7.847	5.786	19.832	0.50	24.26
ATOM	3476	C2*	PCP	401	10.762	6.409	20.931	0.50	39.01
ATOM	3477	O2*	PCP	401	11.609	5.326	21.412	0.50	43.88
ATOM	3479	C3*	PCP	401	11.396	7.674	21.373	0.50	42.14
ATOM	3480	O3*	PCP	401	11.918	7.515	22.681	0.50	44.21
ATOM	3482	N	SER	461	78.844	26.057	14.057	1.00	43.87
ATOM	3484	CA	SER	461	79.399	24.884	13.385	1.00	43.50
ATOM	3485	CB	SER	461	78.488	23.655	13.616	1.00	39.99
ATOM	3486	C	SER	461	79.572	25.181	11.888	1.00	42.14
ATOM	3487	O	SER	461	79.473	24.292	11.038	1.00	40.29
ATOM	3488	N	GLU	462	79.883	26.441	11.594	1.00	43.19
ATOM	3490	CA	GLU	462	80.061	26.951	10.233	1.00	42.77
ATOM	3491	CB	GLU	462	80.303	28.446	10.250	1.00	47.75
ATOM	3492	CG	GLU	462	79.209	29.301	10.860	1.00	60.57
ATOM	3493	CD	GLU	462	79.647	30.752	11.061	1.00	67.56
ATOM	3494	OE1	GLU	462	80.866	31.016	10.994	1.00	67.47
ATOM	3495	OE2	GLU	462	78.764	31.611	11.296	1.00	72.32
ATOM	3496	C	GLU	462	81.207	26.357	9.457	1.00	39.55
ATOM	3497	O	GLU	462	81.051	26.032	8.292	1.00	38.74
ATOM	3498	N	TYR	463	82.375	26.299	10.091	1.00	36.47

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ATOM	3500	CA	TYR	463	83.567	25.806	9.420	1.00	34.19
ATOM	3501	CB	TYR	463	84.702	26.828	9.505	1.00	35.55
ATOM	3502	CG	TYR	463	84.393	28.059	8.675	1.00	42.11
ATOM	3503	CD1	TYR	463	84.004	29.264	9.283	1.00	43.15
ATOM	3504	CE1	TYR	463	83.619	30.361	8.513	1.00	42.40
ATOM	3505	CD2	TYR	463	84.395	27.990	7.280	1.00	39.78
ATOM	3506	CE2	TYR	463	84.012	29.078	6.509	1.00	39.04
ATOM	3507	CZ	TYR	463	83.625	30.256	7.129	1.00	39.86
ATOM	3508	OH	TYR	463	83.260	31.330	6.366	1.00	42.58
ATOM	3510	C	TYR	463	84.055	24.434	9.800	1.00	33.28
ATOM	3511	O	TYR	463	84.739	23.781	9.005	1.00	33.47
ATOM	3512	N	GLU	464	83.695	23.976	10.993	1.00	34.42
ATOM	3514	CA	GLU	464	84.117	22.660	11.444	1.00	36.38
ATOM	3515	CB	GLU	464	85.618	22.663	11.750	1.00	40.90
ATOM	3516	CG	GLU	464	86.041	23.755	12.729	1.00	46.29
ATOM	3517	CD	GLU	464	87.548	23.810	12.943	1.00	51.33
ATOM	3518	OE1	GLU	464	87.970	24.247	14.038	1.00	54.49
ATOM	3519	OE2	GLU	464	88.312	23.430	12.025	1.00	53.18
ATOM	3520	C	GLU	464	83.374	22.224	12.678	1.00	35.64
ATOM	3521	O	GLU	464	83.111	23.052	13.555	1.00	37.40
ATOM	3522	N	LEU	465	82.962	20.955	12.711	1.00	34.21
ATOM	3524	CA	LEU	465	82.267	20.429	13.887	1.00	34.92
ATOM	3525	CB	LEU	465	81.285	19.300	13.542	1.00	31.30
ATOM	3526	CG	LEU	465	80.272	19.381	12.405	1.00	32.22
ATOM	3527	CD1	LEU	465	79.152	18.407	12.720	1.00	21.95
ATOM	3528	CD2	LEU	465	79.738	20.802	12.212	1.00	29.75
ATOM	3529	C	LEU	465	83.326	19.855	14.814	1.00	36.17
ATOM	3530	O	LEU	465	84.473	19.621	14.400	1.00	35.80
ATOM	3531	N	PRO	466	82.970	19.629	16.083	1.00	36.20
ATOM	3532	CD	PRO	466	81.722	20.018	16.758	1.00	38.17
ATOM	3533	CA	PRO	466	83.925	19.072	17.037	1.00	36.06
ATOM	3534	CB	PRO	466	83.132	19.035	18.333	1.00	35.57
ATOM	3535	CG	PRO	466	82.185	20.194	18.171	1.00	38.67
ATOM	3536	C	PRO	466	84.294	17.666	16.605	1.00	37.06
ATOM	3537	O	PRO	466	83.498	16.959	15.979	1.00	34.50
ATOM	3538	N	GLU	467	85.504	17.258	16.936	1.00	39.97
ATOM	3540	CA	GLU	467	85.951	15.932	16.587	1.00	44.69
ATOM	3541	CB	GLU	467	87.412	15.985	16.151	1.00	50.43
ATOM	3542	CG	GLU	467	87.902	14.695	15.518	1.00	60.27
ATOM	3543	CD	GLU	467	89.321	14.796	14.986	1.00	65.75
ATOM	3544	OE1	GLU	467	90.024	15.804	15.269	1.00	64.40
ATOM	3545	OE2	GLU	467	89.726	13.850	14.275	1.00	71.13
ATOM	3546	C	GLU	467	85.775	15.002	17.783	1.00	43.30
ATOM	3547	O	GLU	467	85.888	15.428	18.936	1.00	43.26
ATOM	3548	N	ASP	468	85.433	13.750	17.504	1.00	43.09
ATOM	3550	CA	ASP	468	85.254	12.739	18.545	1.00	44.15
ATOM	3551	CB	ASP	468	83.785	12.614	18.979	1.00	44.54
ATOM	3552	CG	ASP	468	83.574	11.562	20.072	1.00	41.84
ATOM	3553	OD1	ASP	468	82.405	11.244	20.368	1.00	39.81
ATOM	3554	OD2	ASP	468	84.570	11.057	20.636	1.00	42.92
ATOM	3555	C	ASP	468	85.746	11.422	17.970	1.00	44.66
ATOM	3556	O	ASP	468	84.982	10.663	17.368	1.00	44.56
ATOM	3557	N	PRO	469	87.034	11.126	18.176	1.00	44.56
ATOM	3558	CD	PRO	469	87.953	11.959	18.971	1.00	45.43

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ATOM	3559	CA	PRO	469	87.707	9.916	17.707	1.00	43.90
ATOM	3560	CB	PRO	469	89.024	9.959	18.476	1.00	45.66
ATOM	3561	CG	PRO	469	89.300	11.438	18.547	1.00	44.89
ATOM	3562	C	PRO	469	86.934	8.627	17.971	1.00	42.60
ATOM	3563	O	PRO	469	86.935	7.730	17.139	1.00	41.35
ATOM	3564	N	ARG	470	86.229	8.569	19.096	1.00	43.25
ATOM	3566	CA	ARG	470	85.460	7.380	19.470	1.00	44.81
ATOM	3567	CB	ARG	470	84.722	7.612	20.789	1.00	48.36
ATOM	3568	CG	ARG	470	85.579	8.201	21.889	1.00	53.41
ATOM	3569	CD	ARG	470	84.764	8.458	23.138	1.00	55.42
ATOM	3570	NE	ARG	470	83.581	9.261	22.861	1.00	58.57
ATOM	3572	CZ	ARG	470	82.748	9.712	23.791	1.00	62.24
ATOM	3573	NH1	ARG	470	82.972	9.445	25.077	1.00	64.57
ATOM	3576	NH2	ARG	470	81.670	10.398	23.436	1.00	63.66
ATOM	3579	C	ARG	470	84.439	6.924	18.437	1.00	43.69
ATOM	3580	O	ARG	470	84.166	5.735	18.313	1.00	45.68
ATOM	3581	N	TRP	471	83.879	7.866	17.693	1.00	42.41
ATOM	3583	CA	TRP	471	82.851	7.534	16.720	1.00	38.92
ATOM	3584	CB	TRP	471	81.577	8.268	17.095	1.00	35.80
ATOM	3585	CG	TRP	471	80.967	7.741	18.335	1.00	37.13
ATOM	3586	CD2	TRP	471	80.158	6.569	18.443	1.00	37.26
ATOM	3587	CE2	TRP	471	79.723	6.483	19.785	1.00	38.20
ATOM	3588	CE3	TRP	471	79.748	5.582	17.530	1.00	35.59
ATOM	3589	CD1	TRP	471	81.010	8.300	19.584	1.00	36.42
ATOM	3590	NE1	TRP	471	80.260	7.553	20.462	1.00	35.89
ATOM	3592	CZ2	TRP	471	78.896	5.454	20.239	1.00	36.18
ATOM	3593	CZ3	TRP	471	78.934	4.561	17.978	1.00	32.81
ATOM	3594	CH2	TRP	471	78.514	4.505	19.321	1.00	34.82
ATOM	3595	C	TRP	471	83.175	7.845	15.277	1.00	39.77
ATOM	3596	O	TRP	471	82.478	7.391	14.362	1.00	39.56
ATOM	3597	N	GLU	472	84.224	8.628	15.075	1.00	39.37
ATOM	3599	CA	GLU	472	84.605	9.043	13.739	1.00	38.42
ATOM	3600	CB	GLU	472	85.794	9.994	13.812	1.00	37.11
ATOM	3601	CG	GLU	472	85.958	10.849	12.582	1.00	34.11
ATOM	3602	CD	GLU	472	84.772	11.757	12.338	1.00	34.03
ATOM	3603	OE1	GLU	472	84.260	12.348	13.317	1.00	31.87
ATOM	3604	OE2	GLU	472	84.367	11.885	11.163	1.00	32.11
ATOM	3605	C	GLU	472	84.910	7.901	12.791	1.00	39.78
ATOM	3606	O	GLU	472	85.656	6.975	13.128	1.00	41.64
ATOM	3607	N	LEU	473	84.303	7.958	11.610	1.00	37.71
ATOM	3609	CA	LEU	473	84.538	6.957	10.590	1.00	36.94
ATOM	3610	CB	LEU	473	83.258	6.196	10.265	1.00	35.38
ATOM	3611	CG	LEU	473	83.438	5.065	9.236	1.00	37.67
ATOM	3612	CD1	LEU	473	84.070	3.845	9.903	1.00	37.28
ATOM	3613	CD2	LEU	473	82.106	4.687	8.598	1.00	37.87
ATOM	3614	C	LEU	473	85.035	7.664	9.330	1.00	39.31
ATOM	3615	O	LEU	473	84.484	8.697	8.938	1.00	40.55
ATOM	3616	N	PRO	474	86.140	7.164	8.732	1.00	39.20
ATOM	3617	CD	PRO	474	87.052	6.170	9.327	1.00	37.83
ATOM	3618	CA	PRO	474	86.735	7.716	7.513	1.00	38.53
ATOM	3619	CB	PRO	474	87.914	6.777	7.282	1.00	37.16
ATOM	3620	CG	PRO	474	88.355	6.488	8.644	1.00	34.42
ATOM	3621	C	PRO	474	85.733	7.607	6.370	1.00	40.25
ATOM	3622	O	PRO	474	85.220	6.523	6.098	1.00	40.70

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ATOM	3623	N	ARG	475	85.492	8.723	5.685	1.00	41.09
ATOM	3625	CA	ARG	475	84.534	8.746	4.590	1.00	42.26
ATOM	3626	CB	ARG	475	84.487	10.132	3.948	1.00	39.19
ATOM	3627	CG	ARG	475	83.957	11.199	4.876	1.00	35.19
ATOM	3628	CD	ARG	475	84.074	12.593	4.301	1.00	30.76
ATOM	3629	NE	ARG	475	83.796	13.567	5.345	1.00	22.86
ATOM	3631	CZ	ARG	475	82.581	13.898	5.748	1.00	21.99
ATOM	3632	NH1	ARG	475	81.529	13.350	5.165	1.00	23.39
ATOM	3635	NH2	ARG	475	82.412	14.662	6.813	1.00	22.55
ATOM	3638	C	ARG	475	84.838	7.692	3.538	1.00	45.38
ATOM	3639	O	ARG	475	83.927	7.182	2.892	1.00	47.15
ATOM	3640	N	ASP	476	86.106	7.319	3.390	1.00	47.13
ATOM	3642	CA	ASP	476	86.461	6.325	2.387	1.00	51.33
ATOM	3643	CB	ASP	476	87.973	6.294	2.134	1.00	55.23
ATOM	3644	CG	ASP	476	88.768	5.841	3.340	1.00	61.16
ATOM	3645	OD1	ASP	476	88.863	4.617	3.573	1.00	65.55
ATOM	3646	OD2	ASP	476	89.331	6.713	4.036	1.00	65.78
ATOM	3647	C	ASP	476	85.932	4.940	2.746	1.00	52.35
ATOM	3648	O	ASP	476	85.815	4.063	1.885	1.00	55.49
ATOM	3649	N	ARG	477	85.609	4.752	4.021	1.00	50.77
ATOM	3651	CA	ARG	477	85.080	3.482	4.508	1.00	48.65
ATOM	3652	CB	ARG	477	85.612	3.208	5.908	1.00	50.02
ATOM	3653	CG	ARG	477	87.067	2.799	5.881	1.00	55.33
ATOM	3654	CD	ARG	477	87.760	3.030	7.201	1.00	60.38
ATOM	3655	NE	ARG	477	87.238	2.207	8.285	1.00	64.36
ATOM	3657	CZ	ARG	477	87.748	2.203	9.513	1.00	69.16
ATOM	3658	NH1	ARG	477	88.794	2.968	9.814	1.00	70.73
ATOM	3661	NH2	ARG	477	87.190	1.459	10.459	1.00	71.59
ATOM	3664	C	ARG	477	83.546	3.414	4.484	1.00	46.25
ATOM	3665	O	ARG	477	82.957	2.481	5.013	1.00	46.36
ATOM	3666	N	LEU	478	82.913	4.372	3.815	1.00	42.23
ATOM	3668	CA	LEU	478	81.464	4.418	3.743	1.00	38.89
ATOM	3669	CB	LEU	478	80.938	5.537	4.657	1.00	37.17
ATOM	3670	CG	LEU	478	79.418	5.733	4.678	1.00	34.13
ATOM	3671	CD1	LEU	478	78.777	4.723	5.609	1.00	32.24
ATOM	3672	CD2	LEU	478	79.074	7.133	5.101	1.00	33.15
ATOM	3673	C	LEU	478	81.059	4.697	2.303	1.00	38.34
ATOM	3674	O	LEU	478	81.515	5.671	1.711	1.00	40.88
ATOM	3675	N	VAL	479	80.208	3.850	1.738	1.00	37.34
ATOM	3677	CA	VAL	479	79.763	4.042	0.364	1.00	37.61
ATOM	3678	CB	VAL	479	80.105	2.829	-0.563	1.00	36.57
ATOM	3679	CG1	VAL	479	79.647	3.105	-1.994	1.00	31.59
ATOM	3680	CG2	VAL	479	81.608	2.567	-0.561	1.00	36.11
ATOM	3681	C	VAL	479	78.267	4.277	0.375	1.00	39.24
ATOM	3682	O	VAL	479	77.484	3.358	0.619	1.00	39.16
ATOM	3683	N	LEU	480	77.894	5.528	0.142	1.00	41.32
ATOM	3685	CA	LEU	480	76.505	5.960	0.123	1.00	41.60
ATOM	3686	CB	LEU	480	76.446	7.480	-0.008	1.00	41.31
ATOM	3687	CG	LEU	480	77.129	8.257	1.118	1.00	39.82
ATOM	3688	CD1	LEU	480	76.985	9.737	0.856	1.00	37.96
ATOM	3689	CD2	LEU	480	76.512	7.887	2.458	1.00	37.70
ATOM	3690	C	LEU	480	75.733	5.312	-1.015	1.00	41.85
ATOM	3691	O	LEU	480	76.235	5.224	-2.131	1.00	45.02
ATOM	3692	N	GLY	481	74.501	4.897	-0.727	1.00	40.86

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ATOM	3694	CA	GLY	481	73.673	4.247	-1.727	1.00	40.21
ATOM	3695	C	GLY	481	72.270	4.806	-1.873	1.00	39.78
ATOM	3696	O	GLY	481	72.058	6.015	-1.810	1.00	41.68
ATOM	3697	N	LYS	482	71.306	3.914	-2.063	1.00	39.98
ATOM	3699	CA	LYS	482	69.910	4.297	-2.249	1.00	42.13
ATOM	3700	CB	LYS	482	69.061	3.056	-2.566	1.00	42.73
ATOM	3701	C	LYS	482	69.284	5.050	-1.084	1.00	43.13
ATOM	3702	O	LYS	482	69.373	4.625	0.060	1.00	44.49
ATOM	3703	N	PRO	483	68.676	6.204	-1.358	1.00	43.22
ATOM	3704	CD	PRO	483	68.708	6.969	-2.613	1.00	44.40
ATOM	3705	CA	PRO	483	68.044	6.973	-0.290	1.00	45.44
ATOM	3706	CB	PRO	483	67.701	8.295	-0.980	1.00	45.01
ATOM	3707	CG	PRO	483	67.573	7.923	-2.414	1.00	43.95
ATOM	3708	C	PRO	483	66.801	6.261	0.232	1.00	47.67
ATOM	3709	O	PRO	483	66.012	5.725	-0.547	1.00	46.76
ATOM	3710	N	LEU	484	66.650	6.242	1.552	1.00	49.68
ATOM	3712	CA	LEU	484	65.514	5.598	2.196	1.00	54.51
ATOM	3713	CB	LEU	484	65.935	5.026	3.555	1.00	52.70
ATOM	3714	CG	LEU	484	67.132	4.066	3.530	1.00	51.83
ATOM	3715	CD1	LEU	484	67.620	3.766	4.933	1.00	50.19
ATOM	3716	CD2	LEU	484	66.755	2.788	2.825	1.00	52.22
ATOM	3717	C	LEU	484	64.317	6.554	2.357	1.00	58.82
ATOM	3718	O	LEU	484	63.158	6.138	2.244	1.00	60.07
ATOM	3719	N	GLY	485	64.599	7.831	2.609	1.00	61.91
ATOM	3721	CA	GLY	485	63.538	8.810	2.778	1.00	65.89
ATOM	3722	C	GLY	485	64.057	10.167	3.227	1.00	69.46
ATOM	3723	O	GLY	485	65.230	10.301	3.597	1.00	70.65
ATOM	3724	N	GLU	486	63.178	11.165	3.241	1.00	70.72
ATOM	3726	CA	GLU	486	63.563	12.521	3.624	1.00	71.32
ATOM	3727	CB	GLU	486	64.015	13.298	2.389	1.00	73.69
ATOM	3728	C	GLU	486	62.435	13.269	4.312	1.00	70.93
ATOM	3729	O	GLU	486	61.281	12.846	4.275	1.00	71.58
ATOM	3730	N	GLY	487	62.781	14.404	4.909	1.00	70.10
ATOM	3732	CA	GLY	487	61.798	15.211	5.603	1.00	68.11
ATOM	3733	C	GLY	487	62.218	16.669	5.598	1.00	67.97
ATOM	3734	O	GLY	487	62.938	17.109	4.696	1.00	67.68
ATOM	3735	N	ALA	488	61.780	17.409	6.615	1.00	67.26
ATOM	3737	CA	ALA	488	62.106	18.826	6.737	1.00	66.90
ATOM	3738	CB	ALA	488	61.362	19.428	7.909	1.00	68.72
ATOM	3739	C	ALA	488	63.607	19.004	6.921	1.00	67.08
ATOM	3740	O	ALA	488	64.124	18.867	8.037	1.00	65.97
ATOM	3741	N	PHE	489	64.297	19.248	5.806	1.00	66.76
ATOM	3743	CA	PHE	489	65.754	19.439	5.773	1.00	65.91
ATOM	3744	CB	PHE	489	66.134	20.794	6.379	1.00	66.45
ATOM	3745	C	PHE	489	66.563	18.288	6.414	1.00	63.92
ATOM	3746	O	PHE	489	67.622	18.503	7.031	1.00	63.16
ATOM	3747	N	GLY	490	66.067	17.069	6.209	1.00	59.03
ATOM	3749	CA	GLY	490	66.710	15.878	6.720	1.00	51.12
ATOM	3750	C	GLY	490	66.619	14.823	5.638	1.00	48.59
ATOM	3751	O	GLY	490	65.608	14.736	4.938	1.00	45.25
ATOM	3752	N	GLN	491	67.659	14.003	5.525	1.00	48.77
ATOM	3754	CA	GLN	491	67.732	12.951	4.519	1.00	47.40
ATOM	3755	CB	GLN	491	68.529	13.474	3.319	1.00	49.92
ATOM	3756	CG	GLN	491	68.653	12.514	2.155	1.00	56.31

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ATOM	3757	CD	GLN	491	69.604	13.020	1.088	1.00	58.79
ATOM	3758	OE1	GLN	491	70.043	14.171	1.130	1.00	59.63
ATOM	3759	NE2	GLN	491	69.929	12.161	0.122	1.00	59.05
ATOM	3762	C	GLN	491	68.407	11.693	5.086	1.00	44.46
ATOM	3763	O	GLN	491	69.396	11.782	5.806	1.00	44.15
ATOM	3764	N	VAL	492	67.867	10.527	4.752	1.00	42.55
ATOM	3766	CA	VAL	492	68.416	9.247	5.205	1.00	39.22
ATOM	3767	CB	VAL	492	67.375	8.458	6.042	1.00	39.40
ATOM	3768	CG1	VAL	492	67.947	7.127	6.524	1.00	40.17
ATOM	3769	CG2	VAL	492	66.922	9.267	7.210	1.00	36.12
ATOM	3770	C	VAL	492	68.746	8.396	3.975	1.00	37.57
ATOM	3771	O	VAL	492	67.888	8.178	3.115	1.00	35.70
ATOM	3772	N	VAL	493	69.990	7.961	3.845	1.00	36.27
ATOM	3774	CA	VAL	493	70.333	7.127	2.711	1.00	37.61
ATOM	3775	CB	VAL	493	71.237	7.863	1.643	1.00	37.45
ATOM	3776	CG1	VAL	493	70.836	9.319	1.524	1.00	38.29
ATOM	3777	CG2	VAL	493	72.717	7.713	1.943	1.00	36.53
ATOM	3778	C	VAL	493	70.952	5.806	3.156	1.00	37.54
ATOM	3779	O	VAL	493	71.542	5.711	4.233	1.00	37.32
ATOM	3780	N	LEU	494	70.691	4.763	2.380	1.00	37.67
ATOM	3782	CA	LEU	494	71.236	3.450	2.656	1.00	38.41
ATOM	3783	CB	LEU	494	70.482	2.387	1.851	1.00	39.16
ATOM	3784	CG	LEU	494	70.834	0.908	2.021	1.00	36.43
ATOM	3785	CD1	LEU	494	70.809	0.508	3.479	1.00	34.69
ATOM	3786	CD2	LEU	494	69.840	0.086	1.229	1.00	37.48
ATOM	3787	C	LEU	494	72.683	3.541	2.202	1.00	39.30
ATOM	3788	O	LEU	494	72.976	4.201	1.207	1.00	39.21
ATOM	3789	N	ALA	495	73.584	2.922	2.954	1.00	40.08
ATOM	3791	CA	ALA	495	74.996	2.954	2.619	1.00	41.70
ATOM	3792	CB	ALA	495	75.654	4.162	3.283	1.00	41.63
ATOM	3793	C	ALA	495	75.670	1.669	3.080	1.00	43.92
ATOM	3794	O	ALA	495	75.033	0.818	3.711	1.00	45.20
ATOM	3795	N	GLU	496	76.946	1.515	2.731	1.00	44.21
ATOM	3797	CA	GLU	496	77.712	0.347	3.137	1.00	43.44
ATOM	3798	CB	GLU	496	78.046	-0.538	1.943	1.00	45.87
ATOM	3799	CG	GLU	496	76.816	-1.142	1.301	1.00	53.11
ATOM	3800	CD	GLU	496	77.145	-2.262	0.339	1.00	56.68
ATOM	3801	OE1	GLU	496	76.473	-3.316	0.410	1.00	61.87
ATOM	3802	OE2	GLU	496	78.068	-2.091	-0.482	1.00	58.18
ATOM	3803	C	GLU	496	78.973	0.773	3.860	1.00	40.97
ATOM	3804	O	GLU	496	79.835	1.437	3.302	1.00	40.91
ATOM	3805	N	ALA	497	79.036	0.439	5.136	1.00	42.07
ATOM	3807	CA	ALA	497	80.173	0.786	5.959	1.00	43.69
ATOM	3808	CB	ALA	497	79.709	1.104	7.366	1.00	40.90
ATOM	3809	C	ALA	497	81.160	-0.372	5.962	1.00	46.16
ATOM	3810	O	ALA	497	80.764	-1.525	5.814	1.00	46.90
ATOM	3811	N	ILE	498	82.446	-0.059	6.090	1.00	48.78
ATOM	3813	CA	ILE	498	83.494	-1.068	6.114	1.00	49.59
ATOM	3814	CB	ILE	498	84.395	-0.993	4.858	1.00	49.46
ATOM	3815	CG2	ILE	498	85.524	-2.006	4.954	1.00	51.16
ATOM	3816	CG1	ILE	498	83.577	-1.244	3.591	1.00	48.96
ATOM	3817	CD1	ILE	498	82.924	0.009	2.998	1.00	52.50
ATOM	3818	C	ILE	498	84.352	-0.877	7.355	1.00	51.33
ATOM	3819	O	ILE	498	84.818	0.230	7.641	1.00	50.42

ATOM	3820	N	GLY	499	84.506	-1.952	8.119	1.00	53.87
ATOM	3822	CA	GLY	499	85.314	-1.909	9.324	1.00	58.16
ATOM	3823	C	GLY	499	84.759	-1.094	10.483	1.00	62.44
ATOM	3824	O	GLY	499	85.510	-0.400	11.175	1.00	65.17
ATOM	3825	N	LEU	500	83.454	-1.187	10.720	1.00	62.92
ATOM	3827	CA	LEU	500	82.839	-0.453	11.822	1.00	61.93
ATOM	3828	CB	LEU	500	81.339	-0.752	11.888	1.00	58.77
ATOM	3829	CG	LEU	500	80.501	-0.207	10.736	1.00	56.68
ATOM	3830	CD1	LEU	500	79.047	-0.547	10.964	1.00	55.05
ATOM	3831	CD2	LEU	500	80.682	1.298	10.635	1.00	56.30
ATOM	3832	C	LEU	500	83.501	-0.820	13.149	1.00	63.28
ATOM	3833	O	LEU	500	83.623	-2.002	13.487	1.00	64.91
ATOM	3834	N	PRO	505	87.387	-6.451	10.091	1.00	82.92
ATOM	3835	CD	PRO	505	88.522	-6.966	10.874	1.00	83.74
ATOM	3836	CA	PRO	505	87.618	-5.052	9.705	1.00	80.73
ATOM	3837	CB	PRO	505	89.027	-4.770	10.247	1.00	81.95
ATOM	3838	CG	PRO	505	89.655	-6.133	10.342	1.00	83.54
ATOM	3839	C	PRO	505	87.514	-4.794	8.205	1.00	77.60
ATOM	3840	O	PRO	505	87.445	-3.651	7.761	1.00	77.24
ATOM	3841	N	ASN	506	87.488	-5.863	7.424	1.00	75.24
ATOM	3843	CA	ASN	506	87.380	-5.727	5.981	1.00	72.92
ATOM	3844	CB	ASN	506	88.435	-6.589	5.283	1.00	73.87
ATOM	3845	C	ASN	506	85.978	-6.122	5.529	1.00	70.43
ATOM	3846	O	ASN	506	85.719	-6.281	4.340	1.00	70.01
ATOM	3847	N	ARG	507	85.075	-6.273	6.491	1.00	68.31
ATOM	3849	CA	ARG	507	83.697	-6.647	6.200	1.00	65.59
ATOM	3850	CB	ARG	507	83.112	-7.429	7.378	1.00	66.34
ATOM	3851	C	ARG	507	82.846	-5.413	5.941	1.00	62.97
ATOM	3852	O	ARG	507	83.191	-4.313	6.375	1.00	63.16
ATOM	3853	N	VAL	508	81.740	-5.599	5.231	1.00	60.02
ATOM	3855	CA	VAL	508	80.840	-4.495	4.947	1.00	58.59
ATOM	3856	CB	VAL	508	80.532	-4.357	3.439	1.00	58.40
ATOM	3857	CG1	VAL	508	81.813	-4.196	2.658	1.00	61.14
ATOM	3858	CG2	VAL	508	79.751	-5.553	2.938	1.00	61.01
ATOM	3859	C	VAL	508	79.537	-4.682	5.707	1.00	57.24
ATOM	3860	O	VAL	508	79.031	-5.803	5.836	1.00	58.42
ATOM	3861	N	THR	509	79.020	-3.579	6.237	1.00	54.22
ATOM	3863	CA	THR	509	77.769	-3.572	6.973	1.00	48.99
ATOM	3864	CB	THR	509	77.971	-3.100	8.428	1.00	49.59
ATOM	3865	OG1	THR	509	78.932	-3.935	9.082	1.00	51.71
ATOM	3867	CG2	THR	509	76.665	-3.166	9.198	1.00	50.69
ATOM	3868	C	THR	509	76.837	-2.606	6.253	1.00	46.51
ATOM	3869	O	THR	509	77.231	-1.503	5.886	1.00	44.91
ATOM	3870	N	LYS	510	75.628	-3.059	5.966	1.00	45.65
ATOM	3872	CA	LYS	510	74.658	-2.208	5.314	1.00	43.61
ATOM	3873	CB	LYS	510	73.598	-3.058	4.632	1.00	45.46
ATOM	3874	CG	LYS	510	72.845	-2.306	3.568	1.00	54.00
ATOM	3875	CD	LYS	510	73.022	-2.912	2.183	1.00	58.74
ATOM	3876	CE	LYS	510	72.194	-4.184	2.007	1.00	59.63
ATOM	3877	NZ	LYS	510	72.711	-5.323	2.815	1.00	61.62
ATOM	3881	C	LYS	510	74.065	-1.359	6.450	1.00	42.05
ATOM	3882	O	LYS	510	73.566	-1.898	7.439	1.00	41.29
ATOM	3883	N	VAL	511	74.185	-0.038	6.333	1.00	40.14
ATOM	3885	CA	VAL	511	73.719	0.894	7.359	1.00	35.38

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ATOM	3886	CB	VAL	511	74.932	1.554	8.074	1.00	33.16
ATOM	3887	CG1	VAL	511	75.761	0.501	8.795	1.00	29.24
ATOM	3888	CG2	VAL	511	75.804	2.295	7.054	1.00	30.37
ATOM	3889	C	VAL	511	72.856	2.005	6.776	1.00	33.90
ATOM	3890	O	VAL	511	72.722	2.110	5.558	1.00	32.53
ATOM	3891	N	ALA	512	72.261	2.813	7.655	1.00	31.97
ATOM	3893	CA	ALA	512	71.434	3.956	7.248	1.00	31.10
ATOM	3894	CB	ALA	512	70.088	3.945	7.952	1.00	27.38
ATOM	3895	C	ALA	512	72.225	5.186	7.660	1.00	30.49
ATOM	3896	O	ALA	512	72.775	5.235	8.766	1.00	30.10
ATOM	3897	N	VAL	513	72.312	6.162	6.765	1.00	30.50
ATOM	3899	CA	VAL	513	73.064	7.382	7.041	1.00	29.68
ATOM	3900	CB	VAL	513	74.204	7.593	6.015	1.00	28.89
ATOM	3901	CG1	VAL	513	74.966	8.856	6.334	1.00	26.30
ATOM	3902	CG2	VAL	513	75.134	6.389	5.987	1.00	26.66
ATOM	3903	C	VAL	513	72.171	8.607	7.012	1.00	28.50
ATOM	3904	O	VAL	513	71.536	8.893	5.994	1.00	26.27
ATOM	3905	N	LYS	514	72.091	9.282	8.154	1.00	29.18
ATOM	3907	CA	LYS	514	71.307	10.508	8.295	1.00	31.52
ATOM	3908	CB	LYS	514	70.797	10.659	9.728	1.00	33.52
ATOM	3909	CG	LYS	514	69.890	9.540	10.198	1.00	35.67
ATOM	3910	CD	LYS	514	69.439	9.831	11.618	1.00	44.89
ATOM	3911	CE	LYS	514	68.313	8.909	12.060	1.00	51.12
ATOM	3912	NZ	LYS	514	67.029	9.137	11.307	1.00	57.11
ATOM	3916	C	LYS	514	72.233	11.681	7.956	1.00	30.75
ATOM	3917	O	LYS	514	73.390	11.698	8.379	1.00	30.08
ATOM	3918	N	MET	515	71.724	12.651	7.201	1.00	29.45
ATOM	3920	CA	MET	515	72.511	13.814	6.786	1.00	28.74
ATOM	3921	CB	MET	515	73.342	13.466	5.552	1.00	27.72
ATOM	3922	CG	MET	515	72.487	13.034	4.378	1.00	31.56
ATOM	3923	SD	MET	515	73.442	12.549	2.945	1.00	34.98
ATOM	3924	CE	MET	515	73.730	10.878	3.330	1.00	31.23
ATOM	3925	C	MET	515	71.585	14.966	6.444	1.00	27.75
ATOM	3926	O	MET	515	70.369	14.794	6.359	1.00	29.07
ATOM	3927	N	LEU	516	72.152	16.145	6.247	1.00	28.33
ATOM	3929	CA	LEU	516	71.348	17.313	5.912	1.00	31.16
ATOM	3930	CB	LEU	516	72.052	18.605	6.339	1.00	28.70
ATOM	3931	CG	LEU	516	72.312	18.866	7.826	1.00	28.33
ATOM	3932	CD1	LEU	516	73.098	20.156	7.949	1.00	28.45
ATOM	3933	CD2	LEU	516	71.020	18.959	8.604	1.00	21.64
ATOM	3934	C	LEU	516	71.069	17.378	4.421	1.00	33.22
ATOM	3935	O	LEU	516	71.762	16.760	3.619	1.00	35.00
ATOM	3936	N	LYS	517	70.022	18.100	4.061	1.00	34.69
ATOM	3938	CA	LYS	517	69.696	18.286	2.665	1.00	34.20
ATOM	3939	CB	LYS	517	68.194	18.475	2.496	1.00	37.45
ATOM	3940	CG	LYS	517	67.403	17.264	2.950	1.00	43.71
ATOM	3941	CD	LYS	517	66.157	17.072	2.126	1.00	51.25
ATOM	3942	CE	LYS	517	65.123	18.135	2.419	1.00	58.56
ATOM	3943	NZ	LYS	517	64.010	18.049	1.438	1.00	63.12
ATOM	3947	C	LYS	517	70.482	19.533	2.259	1.00	33.81
ATOM	3948	O	LYS	517	70.991	20.244	3.130	1.00	33.17
ATOM	3949	N	SER	518	70.603	19.788	0.959	1.00	33.42
ATOM	3951	CA	SER	518	71.369	20.938	0.472	1.00	33.33
ATOM	3952	CB	SER	518	71.550	20.842	-1.042	1.00	33.23

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ATOM	3953	OG	SER	518	70.306	20.624	-1.678	1.00	38.84
ATOM	3955	C	SER	518	70.794	22.298	0.846	1.00	33.23
ATOM	3956	O	SER	518	71.509	23.305	0.865	1.00	34.14
ATOM	3957	N	ASP	519	69.510	22.313	1.178	1.00	32.77
ATOM	3959	CA	ASP	519	68.825	23.541	1.570	1.00	33.26
ATOM	3960	CB	ASP	519	67.401	23.563	0.995	1.00	35.10
ATOM	3961	CG	ASP	519	66.484	22.503	1.617	1.00	38.98
ATOM	3962	OD1	ASP	519	66.958	21.430	2.042	1.00	37.30
ATOM	3963	OD2	ASP	519	65.261	22.754	1.674	1.00	43.65
ATOM	3964	C	ASP	519	68.793	23.747	3.091	1.00	33.05
ATOM	3965	O	ASP	519	68.114	24.648	3.580	1.00	35.19
ATOM	3966	N	ALA	520	69.538	22.931	3.833	1.00	31.38
ATOM	3968	CA	ALA	520	69.570	23.032	5.293	1.00	29.47
ATOM	3969	CB	ALA	520	70.264	21.830	5.870	1.00	29.74
ATOM	3970	C	ALA	520	70.229	24.301	5.812	1.00	29.83
ATOM	3971	O	ALA	520	71.004	24.952	5.106	1.00	30.23
ATOM	3972	N	THR	521	69.938	24.616	7.071	1.00	31.57
ATOM	3974	CA	THR	521	70.487	25.793	7.742	1.00	34.56
ATOM	3975	CB	THR	521	69.361	26.736	8.302	1.00	38.37
ATOM	3976	OG1	THR	521	68.670	26.082	9.376	1.00	41.75
ATOM	3978	CG2	THR	521	68.357	27.117	7.209	1.00	38.30
ATOM	3979	C	THR	521	71.353	25.363	8.916	1.00	33.22
ATOM	3980	O	THR	521	71.320	24.207	9.327	1.00	32.31
ATOM	3981	N	GLU	522	72.092	26.310	9.479	1.00	34.43
ATOM	3983	CA	GLU	522	72.951	26.042	10.619	1.00	39.53
ATOM	3984	CB	GLU	522	73.634	27.340	11.068	1.00	46.35
ATOM	3985	CG	GLU	522	74.398	27.271	12.402	1.00	58.03
ATOM	3986	CD	GLU	522	75.772	26.603	12.301	1.00	63.14
ATOM	3987	OE1	GLU	522	76.800	27.321	12.404	1.00	61.75
ATOM	3988	OE2	GLU	522	75.824	25.359	12.158	1.00	66.35
ATOM	3989	C	GLU	522	72.130	25.428	11.765	1.00	38.40
ATOM	3990	O	GLU	522	72.642	24.622	12.543	1.00	37.92
ATOM	3991	N	LYS	523	70.853	25.792	11.849	1.00	36.43
ATOM	3993	CA	LYS	523	69.995	25.261	12.893	1.00	36.83
ATOM	3994	CB	LYS	523	68.703	26.065	13.008	1.00	40.88
ATOM	3995	CG	LYS	523	67.793	25.636	14.152	1.00	44.55
ATOM	3996	CD	LYS	523	66.584	24.898	13.607	1.00	52.68
ATOM	3997	CE	LYS	523	65.629	24.483	14.708	1.00	56.04
ATOM	3998	NZ	LYS	523	64.537	23.646	14.123	1.00	58.13
ATOM	4002	C	LYS	523	69.689	23.804	12.601	1.00	35.27
ATOM	4003	O	LYS	523	69.645	22.985	13.513	1.00	36.58
ATOM	4004	N	ASP	524	69.496	23.473	11.326	1.00	32.27
ATOM	4006	CA	ASP	524	69.235	22.089	10.963	1.00	27.18
ATOM	4007	CB	ASP	524	68.952	21.953	9.480	1.00	26.32
ATOM	4008	CG	ASP	524	67.635	22.555	9.089	1.00	25.22
ATOM	4009	OD1	ASP	524	66.662	22.394	9.848	1.00	31.78
ATOM	4010	OD2	ASP	524	67.568	23.190	8.028	1.00	24.00
ATOM	4011	C	ASP	524	70.445	21.268	11.342	1.00	26.83
ATOM	4012	O	ASP	524	70.312	20.165	11.851	1.00	28.65
ATOM	4013	N	LEU	525	71.633	21.827	11.129	1.00	28.69
ATOM	4015	CA	LEU	525	72.872	21.148	11.473	1.00	26.96
ATOM	4016	CB	LEU	525	74.077	21.981	11.049	1.00	22.80
ATOM	4017	CG	LEU	525	75.445	21.355	11.341	1.00	22.32
ATOM	4018	CD1	LEU	525	75.522	19.883	10.858	1.00	18.89

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ATOM	4019	CD2	LEU	525	76.504	22.212	10.704	1.00	17.44
ATOM	4020	C	LEU	525	72.886	20.926	12.980	1.00	28.00
ATOM	4021	O	LEU	525	73.160	19.816	13.462	1.00	28.82
ATOM	4022	N	SER	526	72.567	21.992	13.707	1.00	27.98
ATOM	4024	CA	SER	526	72.496	21.994	15.168	1.00	30.78
ATOM	4025	CB	SER	526	71.939	23.345	15.627	1.00	33.18
ATOM	4026	OG	SER	526	71.624	23.347	17.009	1.00	42.73
ATOM	4028	C	SER	526	71.599	20.865	15.704	1.00	30.56
ATOM	4029	O	SER	526	71.906	20.206	16.716	1.00	31.92
ATOM	4030	N	ASP	527	70.484	20.665	15.018	1.00	28.19
ATOM	4032	CA	ASP	527	69.516	19.651	15.366	1.00	27.41
ATOM	4033	CB	ASP	527	68.207	19.932	14.632	1.00	27.63
ATOM	4034	CG	ASP	527	67.492	21.172	15.149	1.00	27.37
ATOM	4035	OD1	ASP	527	67.870	21.728	16.211	1.00	26.70
ATOM	4036	OD2	ASP	527	66.525	21.579	14.487	1.00	33.80
ATOM	4037	C	ASP	527	70.007	18.241	15.063	1.00	27.36
ATOM	4038	O	ASP	527	69.722	17.309	15.816	1.00	30.13
ATOM	4039	N	LEU	528	70.716	18.077	13.952	1.00	25.76
ATOM	4041	CA	LEU	528	71.245	16.765	13.588	1.00	25.29
ATOM	4042	CB	LEU	528	71.777	16.771	12.143	1.00	23.65
ATOM	4043	CG	LEU	528	72.283	15.432	11.574	1.00	25.86
ATOM	4044	CD1	LEU	528	71.234	14.341	11.770	1.00	23.35
ATOM	4045	CD2	LEU	528	72.652	15.566	10.102	1.00	17.46
ATOM	4046	C	LEU	528	72.351	16.368	14.578	1.00	25.66
ATOM	4047	C	LEU	528	72.418	15.210	15.015	1.00	24.02
ATOM	4048	N	ILE	529	73.200	17.338	14.934	1.00	26.36
ATOM	4050	CA	ILE	529	74.304	17.130	15.886	1.00	26.17
ATOM	4051	CB	ILE	529	75.192	18.381	16.003	1.00	22.72
ATOM	4052	CG2	ILE	529	76.250	18.180	17.057	1.00	21.32
ATOM	4053	CG1	ILE	529	75.876	18.666	14.685	1.00	20.71
ATOM	4054	CD1	ILE	529	76.621	19.965	14.675	1.00	25.60
ATOM	4055	C	ILE	529	73.756	16.835	17.283	1.00	29.87
ATOM	4056	O	ILE	529	74.253	15.948	17.977	1.00	32.20
ATOM	4057	N	SER	530	72.741	17.591	17.693	1.00	28.63
ATOM	4059	CA	SER	530	72.143	17.381	18.991	1.00	32.21
ATOM	4060	CB	SER	530	71.031	18.399	19.231	1.00	37.45
ATOM	4061	OG	SER	530	70.065	18.342	18.195	1.00	49.52
ATOM	4063	C	SER	530	71.598	15.956	19.075	1.00	30.96
ATOM	4064	O	SER	530	71.728	15.301	20.105	1.00	33.05
ATOM	4065	N	GLU	531	70.996	15.476	17.996	1.00	29.13
ATOM	4067	CA	GLU	531	70.468	14.117	17.987	1.00	29.84
ATOM	4068	CB	GLU	531	69.672	13.847	16.709	1.00	30.29
ATOM	4069	CG	GLU	531	69.093	12.445	16.666	1.00	27.39
ATOM	4070	CD	GLU	531	68.521	12.074	15.331	1.00	31.34
ATOM	4071	OE1	GLU	531	67.929	10.981	15.228	1.00	35.90
ATOM	4072	OE2	GLU	531	68.660	12.860	14.376	1.00	38.37
ATOM	4073	C	GLU	531	71.600	13.081	18.109	1.00	28.48
ATOM	4074	O	GLU	531	71.468	12.094	18.822	1.00	28.17
ATOM	4075	N	MET	532	72.682	13.281	17.364	1.00	28.12
ATOM	4077	CA	MET	532	73.832	12.376	17.409	1.00	27.64
ATOM	4078	CB	MET	532	74.953	12.899	16.499	1.00	26.47
ATOM	4079	CG	MET	532	76.267	12.125	16.601	1.00	22.25
ATOM	4080	SD	MET	532	77.406	12.610	15.286	1.00	30.32
ATOM	4081	CE	MET	532	77.613	14.366	15.661	1.00	20.92

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ATOM	4082	C	MET	532	74.339	12.328	18.832	1.00	27.87	
ATOM	4083	O	MET	532	74.640	11.267	19.364	1.00	30.31	
ATOM	4084	N	GLU	533	74.439	13.497	19.442	1.00	27.08	
ATOM	4086	CA	GLU	533	74.906	13.594	20.802	1.00	28.50	
ATOM	4087	CB	GLU	533	75.071	15.064	21.177	1.00	29.09	
ATOM	4088	CG	GLU	533	76.216	15.745	20.433	1.00	28.90	
ATOM	4089	CD	GLU	533	77.564	15.070	20.661	1.00	31.08	
ATOM	4090	OE1	GLU	533	78.001	14.969	21.823	1.00	34.15	
ATOM	4091	OE2	GLU	533	78.202	14.643	19.678	1.00	33.60	
ATOM	4092	C	GLU	533	73.981	12.850	21.774	1.00	29.91	
ATOM	4093	O	GLU	533	74.455	12.093	22.637	1.00	29.73	
ATOM	4094	N	MET	534	72.670	13.014	21.588	1.00	29.70	
ATOM	4096	CA	MET	534	71.692	12.346	22.444	1.00	27.97	
ATOM	4097	CB	MET	534	70.258	12.751	22.082	1.00	28.95	
ATOM	4098	CG	MET	534	69.311	12.594	23.278	0.50	29.62	PRT1
ATOM	4099	SD	MET	534	67.538	12.682	22.961	0.50	29.87	PRT1
ATOM	4100	CE	MET	534	67.269	14.452	22.795	0.50	31.07	PRT1
ATOM	4101	C	MET	534	71.855	10.821	22.362	1.00	28.36	
ATOM	4102	O	MET	534	71.833	10.143	23.386	1.00	27.02	
ATOM	4103	N	MET	535	72.048	10.297	21.151	1.00	26.96	
ATOM	4105	CA	MET	535	72.239	8.861	20.947	1.00	26.63	
ATOM	4106	CB	MET	535	72.347	8.521	19.456	1.00	24.67	
ATOM	4107	CG	MET	535	71.089	8.778	18.659	1.00	23.15	
ATOM	4108	SD	MET	535	71.160	8.062	17.011	1.00	24.57	
ATOM	4109	CE	MET	535	71.251	9.486	16.023	1.00	24.79	
ATOM	4110	C	MET	535	73.498	8.390	21.569	1.00	27.66	
ATOM	4111	O	MET	535	73.564	7.259	22.164	1.00	28.93	
ATOM	4112	N	LYS	536	74.515	9.246	21.698	1.00	29.13	
ATOM	4114	CA	LYS	536	75.757	8.918	22.392	1.00	30.50	
ATOM	4115	CB	LYS	536	76.812	9.985	22.131	1.00	29.15	
ATOM	4116	CG	LYS	536	77.499	9.883	20.802	1.00	27.71	
ATOM	4117	CD	LYS	536	78.377	11.100	20.615	1.00	28.12	
ATOM	4118	CE	LYS	536	79.085	11.096	19.279	1.00	26.89	
ATOM	4119	NZ	LYS	536	79.688	12.436	19.077	1.00	27.54	
ATOM	4123	C	LYS	536	75.480	8.836	23.892	1.00	31.92	
ATOM	4124	O	LYS	536	75.921	7.908	24.559	1.00	31.19	
ATOM	4125	N	MET	537	74.742	9.814	24.409	1.00	34.02	
ATOM	4127	CA	MET	537	74.384	9.881	25.822	1.00	36.35	
ATOM	4128	CB	MET	537	73.648	11.197	26.083	1.00	43.33	
ATOM	4129	CG	MET	537	73.096	11.376	27.507	1.00	54.60	
ATOM	4130	SD	MET	537	71.426	10.674	27.856	1.00	67.38	
ATOM	4131	CE	MET	537	71.684	9.813	29.440	1.00	62.03	
ATOM	4132	C	MET	537	73.507	8.705	26.253	1.00	34.53	
ATOM	4133	O	MET	537	73.744	8.069	27.275	1.00	36.76	
ATOM	4134	N	ILE	538	72.496	8.425	25.454	1.00	32.24	
ATOM	4136	CA	ILE	538	71.568	7.367	25.757	1.00	29.88	
ATOM	4137	CB	ILE	538	70.396	7.384	24.757	1.00	26.98	
ATOM	4138	CG2	ILE	538	69.582	6.096	24.842	1.00	27.93	
ATOM	4139	CG1	ILE	538	69.527	8.614	25.036	1.00	22.58	
ATOM	4140	CD1	ILE	538	68.399	8.787	24.058	1.00	24.58	
ATOM	4141	C	ILE	538	72.236	6.006	25.804	1.00	31.83	
ATOM	4142	O	ILE	538	71.983	5.227	26.713	1.00	36.32	
ATOM	4143	N	GLY	539	73.102	5.718	24.848	1.00	32.45	
ATOM	4145	CA	GLY	539	73.744	4.422	24.850	1.00	32.13	

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ATOM	4146	C	GLY	539	72.974	3.380	24.056	1.00	33.83
ATOM	4147	O	GLY	539	71.876	3.654	23.530	1.00	33.75
ATOM	4148	N	LYS	540	73.539	2.173	24.010	1.00	33.36
ATOM	4150	CA	LYS	540	72.980	1.054	23.256	1.00	37.04
ATOM	4151	CB	LYS	540	74.110	0.181	22.709	1.00	39.21
ATOM	4152	CG	LYS	540	74.865	0.893	21.623	1.00	48.72
ATOM	4153	CD	LYS	540	75.818	0.009	20.850	1.00	56.84
ATOM	4154	CE	LYS	540	76.225	0.693	19.516	1.00	62.14
ATOM	4155	NZ	LYS	540	77.252	-0.102	18.805	1.00	71.02
ATOM	4159	C	LYS	540	71.938	0.162	23.901	1.00	36.51
ATOM	4160	O	LYS	540	71.963	-0.096	25.113	1.00	38.52
ATOM	4161	N	HIS	541	71.017	-0.295	23.058	1.00	32.98
ATOM	4163	CA	HIS	541	69.963	-1.230	23.424	1.00	31.20
ATOM	4164	CB	HIS	541	68.779	-0.561	24.095	1.00	30.35
ATOM	4165	CG	HIS	541	67.815	-1.540	24.694	1.00	32.56
ATOM	4166	CD2	HIS	541	67.737	-2.058	25.941	1.00	32.45
ATOM	4167	ND1	HIS	541	66.795	-2.124	23.974	1.00	29.22
ATOM	4169	CE1	HIS	541	66.134	-2.965	24.753	1.00	31.56
ATOM	4170	NE2	HIS	541	66.679	-2.932	25.957	1.00	32.22
ATOM	4172	C	HIS	541	69.509	-1.937	22.152	1.00	32.00
ATOM	4173	O	HIS	541	69.409	-1.324	21.095	1.00	32.84
ATOM	4174	N	LYS	542	69.187	-3.222	22.273	1.00	33.61
ATOM	4176	CA	LYS	542	68.786	-4.061	21.154	1.00	31.54
ATOM	4177	CB	LYS	542	68.653	-5.516	21.596	1.00	33.94
ATOM	4178	CG	LYS	542	68.322	-6.451	20.437	1.00	42.34
ATOM	4179	CD	LYS	542	68.083	-7.885	20.856	1.00	47.57
ATOM	4180	CE	LYS	542	67.634	-8.726	19.658	1.00	52.70
ATOM	4181	NZ	LYS	542	67.402	-10.146	20.023	1.00	59.51
ATOM	4185	C	LYS	542	67.495	-3.611	20.487	1.00	29.57
ATOM	4186	O	LYS	542	67.268	-3.884	19.305	1.00	27.99
ATOM	4187	N	ASN	543	66.649	-2.931	21.253	1.00	28.32
ATOM	4189	CA	ASN	543	65.378	-2.476	20.714	1.00	28.86
ATOM	4190	CB	ASN	543	64.231	-2.947	21.601	1.00	29.33
ATOM	4191	CG	ASN	543	64.247	-4.452	21.811	1.00	29.64
ATOM	4192	OD1	ASN	543	64.437	-4.926	22.930	1.00	33.86
ATOM	4193	ND2	ASN	543	64.106	-5.206	20.732	1.00	28.02
ATOM	4196	C	ASN	543	65.252	-0.983	20.378	1.00	29.69
ATOM	4197	O	ASN	543	64.159	-0.413	20.457	1.00	30.02
ATOM	4198	N	ILE	544	66.372	-0.357	20.011	1.00	27.35
ATOM	4200	CA	ILE	544	66.382	1.046	19.593	1.00	25.95
ATOM	4201	CB	ILE	544	66.898	2.030	20.706	1.00	25.56
ATOM	4202	CG2	ILE	544	66.148	1.819	22.037	1.00	21.06
ATOM	4203	CG1	ILE	544	68.406	1.901	20.902	1.00	25.61
ATOM	4204	CD1	ILE	544	68.952	2.818	21.976	1.00	25.89
ATOM	4205	C	ILE	544	67.341	1.083	18.399	1.00	25.97
ATOM	4206	O	ILE	544	68.126	0.152	18.227	1.00	25.69
ATOM	4207	N	ILE	545	67.226	2.095	17.537	1.00	27.27
ATOM	4209	CA	ILE	545	68.129	2.243	16.384	1.00	27.02
ATOM	4210	CB	ILE	545	67.541	3.194	15.307	1.00	27.30
ATOM	4211	CG2	ILE	545	68.592	3.553	14.269	1.00	26.52
ATOM	4212	CG1	ILE	545	66.309	2.570	14.638	1.00	22.63
ATOM	4213	CD1	ILE	545	66.605	1.447	13.665	1.00	17.57
ATOM	4214	C	ILE	545	69.383	2.873	16.979	1.00	28.55
ATOM	4215	O	ILE	545	69.346	4.014	17.451	1.00	29.47

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ATOM	4216	N	ASN	546	70.482	2.123	16.965	1.00	30.90
ATOM	4218	CA	ASN	546	71.748	2.564	17.560	1.00	29.56
ATOM	4219	CB	ASN	546	72.497	1.365	18.159	1.00	26.32
ATOM	4220	CG	ASN	546	71.732	0.695	19.281	1.00	23.81
ATOM	4221	OD1	ASN	546	71.580	1.252	20.362	1.00	27.34
ATOM	4222	ND2	ASN	546	71.267	-0.515	19.039	1.00	23.49
ATOM	4225	C	ASN	546	72.700	3.330	16.653	1.00	30.99
ATOM	4226	O	ASN	546	72.679	3.169	15.430	1.00	30.98
ATOM	4227	N	LEU	547	73.543	4.148	17.286	1.00	32.29
ATOM	4229	CA	LEU	547	74.570	4.948	16.610	1.00	30.93
ATOM	4230	CB	LEU	547	75.043	6.076	17.542	1.00	25.97
ATOM	4231	CG	LEU	547	76.075	7.088	17.021	1.00	22.12
ATOM	4232	CD1	LEU	547	75.553	7.815	15.765	1.00	22.10
ATOM	4233	CD2	LEU	547	76.415	8.089	18.112	1.00	18.67
ATOM	4234	C	LEU	547	75.756	4.039	16.264	1.00	30.70
ATOM	4235	O	LEU	547	76.284	3.361	17.137	1.00	34.46
ATOM	4236	N	LEU	548	76.141	3.993	14.992	1.00	30.97
ATOM	4238	CA	LEU	548	77.262	3.165	14.562	1.00	30.73
ATOM	4239	CB	LEU	548	76.929	2.406	13.281	1.00	29.24
ATOM	4240	CG	LEU	548	75.788	1.394	13.371	1.00	28.77
ATOM	4241	CD1	LEU	548	75.924	0.460	12.209	1.00	26.55
ATOM	4242	CD2	LEU	548	75.839	0.616	14.683	1.00	23.48
ATOM	4243	C	LEU	548	78.522	3.982	14.347	1.00	33.00
ATOM	4244	O	LEU	548	79.640	3.500	14.558	1.00	35.92
ATOM	4245	N	GLY	549	78.351	5.215	13.901	1.00	32.52
ATOM	4247	CA	GLY	549	79.503	6.051	13.673	1.00	32.76
ATOM	4248	C	GLY	549	79.092	7.411	13.180	1.00	33.72
ATOM	4249	O	GLY	549	77.895	7.707	13.092	1.00	35.01
ATOM	4250	N	ALA	550	80.089	8.226	12.840	1.00	33.47
ATOM	4252	CA	ALA	550	79.848	9.566	12.337	1.00	30.69
ATOM	4253	CB	ALA	550	79.555	10.509	13.497	1.00	28.66
ATOM	4254	C	ALA	550	81.022	10.099	11.523	1.00	30.41
ATOM	4255	O	ALA	550	82.181	9.780	11.808	1.00	29.13
ATOM	4256	N	CYS	551	80.695	10.817	10.446	1.00	30.29
ATOM	4258	CA	CYS	551	81.675	11.490	9.584	1.00	28.44
ATOM	4259	CB	CYS	551	81.432	11.214	8.096	1.00	27.25
ATOM	4260	SG	CYS	551	81.639	9.508	7.566	1.00	28.89
ATOM	4261	C	CYS	551	81.337	12.950	9.883	1.00	27.07
ATOM	4262	O	CYS	551	80.293	13.441	9.467	1.00	29.86
ATOM	4263	N	THR	552	82.184	13.616	10.658	1.00	25.10
ATOM	4265	CA	THR	552	81.952	14.997	11.047	1.00	24.37
ATOM	4266	CB	THR	552	81.959	15.091	12.569	1.00	27.67
ATOM	4267	OG1	THR	552	83.271	14.760	13.052	1.00	26.11
ATOM	4269	CG2	THR	552	80.951	14.120	13.164	1.00	30.41
ATOM	4270	C	THR	552	83.003	15.980	10.557	1.00	24.51
ATOM	4271	O	THR	552	82.804	17.194	10.604	1.00	21.56
ATOM	4272	N	GLN	553	84.151	15.441	10.162	1.00	27.13
ATOM	4274	CA	GLN	553	85.284	16.243	9.710	1.00	26.64
ATOM	4275	CB	GLN	553	86.592	15.679	10.283	1.00	25.24
ATOM	4276	CG	GLN	553	86.641	15.561	11.809	1.00	22.38
ATOM	4277	CD	GLN	553	86.464	16.897	12.515	1.00	24.04
ATOM	4278	OE1	GLN	553	87.267	17.815	12.344	1.00	31.50
ATOM	4279	NE2	GLN	553	85.403	17.017	13.304	1.00	21.59
ATOM	4282	C	GLN	553	85.384	16.276	8.206	1.00	28.02

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ATOM	4283	O	GLN	553	85.069	15.293	7.537	1.00	30.20
ATOM	4284	N	ASP	554	85.794	17.430	7.695	1.00	28.08
ATOM	4286	CA	ASP	554	86.000	17.652	6.263	1.00	30.14
ATOM	4287	CB	ASP	554	87.330	17.034	5.833	1.00	29.82
ATOM	4288	CG	ASP	554	88.451	17.470	6.707	1.00	31.79
ATOM	4289	OD1	ASP	554	88.699	18.666	6.767	1.00	36.45
ATOM	4290	OD2	ASP	554	89.066	16.623	7.364	1.00	33.06
ATOM	4291	C	ASP	554	84.895	17.217	5.317	1.00	29.52
ATOM	4292	O	ASP	554	85.128	16.411	4.424	1.00	33.67
ATOM	4293	N	GLY	555	83.709	17.793	5.488	1.00	29.02
ATOM	4295	CA	GLY	555	82.586	17.476	4.621	1.00	26.05
ATOM	4296	C	GLY	555	81.286	17.447	5.405	1.00	23.80
ATOM	4297	O	GLY	555	81.269	17.751	6.597	1.00	24.09
ATOM	4298	N	PRO	556	80.175	17.117	4.740	1.00	23.29
ATOM	4299	CD	PRO	556	80.094	16.804	3.304	1.00	18.93
ATOM	4300	CA	PRO	556	78.860	17.045	5.378	1.00	23.45
ATOM	4301	CB	PRO	556	77.943	16.643	4.226	1.00	22.35
ATOM	4302	CG	PRO	556	78.889	15.931	3.261	1.00	24.94
ATOM	4303	C	PRO	556	78.806	16.019	6.503	1.00	26.66
ATOM	4304	O	PRO	556	79.488	14.984	6.464	1.00	27.76
ATOM	4305	N	LEU	557	78.006	16.324	7.522	1.00	29.14
ATOM	4307	CA	LEU	557	77.842	15.440	8.676	1.00	30.83
ATOM	4308	CB	LEU	557	77.173	16.181	9.842	1.00	28.40
ATOM	4309	CG	LEU	557	76.775	15.393	11.097	1.00	22.93
ATOM	4310	CD1	LEU	557	77.989	14.897	11.835	1.00	23.02
ATOM	4311	CD2	LEU	557	75.970	16.285	11.984	1.00	23.53
ATOM	4312	C	LEU	557	77.028	14.200	8.321	1.00	31.04
ATOM	4313	O	LEU	557	75.968	14.293	7.694	1.00	31.89
ATOM	4314	N	TYR	558	77.552	13.041	8.700	1.00	29.88
ATOM	4316	CA	TYR	558	76.891	11.773	8.460	1.00	27.80
ATOM	4317	CB	TYR	558	77.741	10.878	7.562	1.00	28.04
ATOM	4318	CG	TYR	558	77.895	11.339	6.122	1.00	29.98
ATOM	4319	CD1	TYR	558	78.843	10.751	5.289	1.00	31.81
ATOM	4320	CE1	TYR	558	78.980	11.140	3.956	1.00	32.22
ATOM	4321	CD2	TYR	558	77.086	12.335	5.584	1.00	31.50
ATOM	4322	CE2	TYR	558	77.214	12.729	4.256	1.00	31.57
ATOM	4323	CZ	TYR	558	78.166	12.125	3.449	1.00	32.04
ATOM	4324	OH	TYR	558	78.317	12.511	2.134	1.00	33.34
ATOM	4326	C	TYR	558	76.715	11.099	9.809	1.00	27.34
ATOM	4327	O	TYR	558	77.678	10.937	10.558	1.00	25.80
ATOM	4328	N	VAL	559	75.464	10.798	10.147	1.00	28.06
ATOM	4330	CA	VAL	559	75.118	10.118	11.394	1.00	26.67
ATOM	4331	CB	VAL	559	73.930	10.816	12.129	1.00	26.22
ATOM	4332	CG1	VAL	559	73.590	10.079	13.425	1.00	22.58
ATOM	4333	CG2	VAL	559	74.298	12.278	12.440	1.00	23.09
ATOM	4334	C	VAL	559	74.745	8.715	10.943	1.00	24.32
ATOM	4335	O	VAL	559	73.665	8.464	10.412	1.00	26.37
ATOM	4336	N	ILE	560	75.689	7.815	11.095	1.00	23.63
ATOM	4338	CA	ILE	560	75.514	6.448	10.664	1.00	24.67
ATOM	4339	CB	ILE	560	76.901	5.859	10.299	1.00	24.62
ATOM	4340	CG2	ILE	560	76.753	4.507	9.646	1.00	30.13
ATOM	4341	CG1	ILE	560	77.627	6.810	9.326	1.00	21.87
ATOM	4342	CD1	ILE	560	79.114	6.538	9.162	1.00	22.25
ATOM	4343	C	ILE	560	74.814	5.621	11.737	1.00	27.30

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ATOM	4344	O	ILE	560	75.306	5.505	12.865	1.00	28.80
ATOM	4345	N	VAL	561	73.641	5.090	11.406	1.00	26.80
ATOM	4347	CA	VAL	561	72.894	4.272	12.352	1.00	26.16
ATOM	4348	CB	VAL	561	71.572	4.953	12.810	1.00	24.10
ATOM	4349	CG1	VAL	561	71.866	6.208	13.599	1.00	24.11
ATOM	4350	CG2	VAL	561	70.676	5.254	11.625	1.00	21.97
ATOM	4351	C	VAL	561	72.572	2.901	11.761	1.00	27.98
ATOM	4352	O	VAL	561	72.853	2.632	10.584	1.00	26.49
ATOM	4353	N	GLU	562	71.998	2.039	12.599	1.00	28.86
ATOM	4355	CA	GLU	562	71.605	0.685	12.219	1.00	28.23
ATOM	4356	CB	GLU	562	71.090	-0.068	13.440	1.00	25.86
ATOM	4357	CG	GLU	562	72.170	-0.392	14.424	1.00	27.04
ATOM	4358	CD	GLU	562	71.641	-0.969	15.714	1.00	28.37
ATOM	4359	OE1	GLU	562	72.389	-1.714	16.372	1.00	33.36
ATOM	4360	OE2	GLU	562	70.491	-0.665	16.092	1.00	31.60
ATOM	4361	C	GLU	562	70.529	0.720	11.171	1.00	29.67
ATOM	4362	O	GLU	562	69.581	1.489	11.287	1.00	32.53
ATOM	4363	N	TYR	563	70.666	-0.126	10.162	1.00	30.70
ATOM	4365	CA	TYR	563	69.699	-0.209	9.083	1.00	30.65
ATOM	4366	CB	TYR	563	70.419	-0.621	7.801	1.00	30.83
ATOM	4367	CG	TYR	563	69.510	-0.905	6.633	1.00	32.10
ATOM	4368	CD1	TYR	563	68.545	0.018	6.236	1.00	33.24
ATOM	4369	CE1	TYR	563	67.715	-0.227	5.160	1.00	34.65
ATOM	4370	CD2	TYR	563	69.609	-2.098	5.922	1.00	31.04
ATOM	4371	CE2	TYR	563	68.779	-2.353	4.838	1.00	33.12
ATOM	4372	CZ	TYR	563	67.831	-1.413	4.470	1.00	34.22
ATOM	4373	CH	TYR	563	67.002	-1.650	3.400	1.00	34.76
ATOM	4375	C	TYR	563	68.592	-1.223	9.406	1.00	34.39
ATOM	4376	O	TYR	563	68.855	-2.325	9.884	1.00	34.87
ATOM	4377	N	ALA	564	67.356	-0.861	9.091	1.00	35.49
ATOM	4379	CA	ALA	564	66.212	-1.726	9.324	1.00	35.41
ATOM	4380	CB	ALA	564	65.213	-1.000	10.210	1.00	35.93
ATOM	4381	C	ALA	564	65.585	-2.056	7.962	1.00	37.19
ATOM	4382	O	ALA	564	64.789	-1.276	7.434	1.00	38.08
ATOM	4383	N	SER	565	65.931	-3.211	7.401	1.00	37.14
ATOM	4385	CA	SER	565	65.433	-3.616	6.080	1.00	36.83
ATOM	4386	CB	SER	565	66.151	-4.881	5.614	1.00	35.24
ATOM	4387	OG	SER	565	66.105	-5.873	6.619	1.00	34.96
ATOM	4389	C	SER	565	63.932	-3.782	5.886	1.00	38.65
ATOM	4390	O	SER	565	63.428	-3.617	4.760	1.00	37.80
ATOM	4391	N	LYS	566	63.212	-4.077	6.964	1.00	38.96
ATOM	4393	CA	LYS	566	61.772	-4.271	6.851	1.00	37.83
ATOM	4394	CB	LYS	566	61.357	-5.495	7.655	1.00	39.07
ATOM	4395	CG	LYS	566	61.954	-6.765	7.078	1.00	43.73
ATOM	4396	CD	LYS	566	61.813	-7.950	7.996	1.00	47.07
ATOM	4397	CE	LYS	566	62.258	-9.216	7.299	1.00	47.77
ATOM	4398	NZ	LYS	566	62.361	-10.326	8.278	1.00	51.48
ATOM	4402	C	LYS	566	60.899	-3.050	7.165	1.00	37.53
ATOM	4403	O	LYS	566	59.702	-3.180	7.442	1.00	38.55
ATOM	4404	N	GLY	567	61.496	-1.866	7.066	1.00	35.23
ATOM	4406	CA	GLY	567	60.788	-0.627	7.305	1.00	33.64
ATOM	4407	C	GLY	567	60.120	-0.485	8.656	1.00	33.24
ATOM	4408	O	GLY	567	60.518	-1.133	9.627	1.00	33.80
ATOM	4409	N	ASN	568	59.120	0.389	8.716	1.00	31.65

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ATOM	4411	CA	ASN	568	58.407	0.623	9.952	1.00	33.38
ATOM	4412	CB	ASN	568	57.831	2.055	10.025	1.00	37.10
ATOM	4413	CG	ASN	568	56.624	2.272	9.116	1.00	37.78
ATOM	4414	OD1	ASN	568	55.552	1.708	9.337	1.00	41.15
ATOM	4415	ND2	ASN	568	56.780	3.147	8.124	1.00	35.74
ATOM	4418	C	ASN	568	57.357	-0.435	10.263	1.00	33.33
ATOM	4419	O	ASN	568	56.917	-1.178	9.384	1.00	32.54
ATOM	4420	N	LEU	569	56.971	-0.490	11.532	1.00	33.35
ATOM	4422	CA	LEU	569	56.004	-1.455	12.040	1.00	32.38
ATOM	4423	CB	LEU	569	55.838	-1.263	13.552	1.00	27.50
ATOM	4424	CG	LEU	569	54.954	-2.259	14.291	1.00	26.34
ATOM	4425	CD1	LEU	569	55.452	-3.671	14.007	1.00	24.19
ATOM	4426	CD2	LEU	569	54.968	-1.951	15.787	1.00	21.44
ATOM	4427	C	LEU	569	54.641	-1.433	11.355	1.00	33.35
ATOM	4428	O	LEU	569	54.060	-2.484	11.095	1.00	34.99
ATOM	4429	N	ARG	570	54.130	-0.239	11.083	1.00	34.36
ATOM	4431	CA	ARG	570	52.827	-0.091	10.445	1.00	36.82
ATOM	4432	CB	ARG	570	52.548	1.393	10.188	1.00	37.28
ATOM	4433	CG	ARG	570	51.210	1.689	9.539	1.00	43.90
ATOM	4434	CD	ARG	570	51.212	3.099	8.967	1.00	50.39
ATOM	4435	NE	ARG	570	52.273	3.268	7.973	1.00	54.99
ATOM	4437	CZ	ARG	570	53.075	4.328	7.887	1.00	54.96
ATOM	4438	NH1	ARG	570	52.947	5.343	8.735	1.00	54.71
ATOM	4441	NH2	ARG	570	54.030	4.357	6.966	1.00	56.12
ATOM	4444	C	ARG	570	52.818	-0.877	9.133	1.00	36.53
ATOM	4445	O	ARG	570	51.968	-1.737	8.909	1.00	34.68
ATOM	4446	N	GLU	571	53.830	-0.611	8.320	1.00	37.14
ATOM	4448	CA	GLU	571	53.954	-1.253	7.031	1.00	37.94
ATOM	4449	CB	GLU	571	55.126	-0.558	6.274	1.00	39.71
ATOM	4450	CG	GLU	571	54.834	0.916	6.062	1.00	44.69
ATOM	4451	CD	GLU	571	55.934	1.665	5.346	1.00	52.22
ATOM	4452	OE1	GLU	571	57.098	1.196	5.358	1.00	54.87
ATOM	4453	OE2	GLU	571	55.629	2.743	4.777	1.00	56.37
ATOM	4454	C	GLU	571	54.258	-2.744	7.164	1.00	36.53
ATOM	4455	O	GLU	571	53.692	-3.550	6.426	1.00	36.35
ATOM	4456	N	TYR	572	55.105	-3.105	8.120	1.00	35.77
ATOM	4458	CA	TYR	572	55.456	-4.499	8.371	1.00	36.28
ATOM	4459	CB	TYR	572	56.446	-4.555	9.534	1.00	30.27
ATOM	4460	CG	TYR	572	56.859	-5.925	10.006	1.00	31.65
ATOM	4461	CD1	TYR	572	57.889	-6.626	9.371	1.00	29.40
ATOM	4462	CE1	TYR	572	58.354	-7.839	9.883	1.00	29.32
ATOM	4463	CD2	TYR	572	56.292	-6.480	11.161	1.00	35.17
ATOM	4464	CE2	TYR	572	56.749	-7.696	11.680	1.00	33.08
ATOM	4465	CZ	TYR	572	57.780	-8.366	11.038	1.00	35.15
ATOM	4466	OH	TYR	572	58.234	-9.559	11.558	1.00	36.91
ATOM	4468	C	TYR	572	54.189	-5.321	8.672	1.00	37.70
ATOM	4469	O	TYR	572	53.942	-6.369	8.068	1.00	36.82
ATOM	4470	N	LEU	573	53.368	-4.799	9.576	1.00	37.64
ATOM	4472	CA	LEU	573	52.126	-5.442	9.970	1.00	36.03
ATOM	4473	CB	LEU	573	51.497	-4.659	11.122	1.00	36.17
ATOM	4474	CG	LEU	573	52.257	-4.641	12.445	1.00	36.39
ATOM	4475	CD1	LEU	573	51.590	-3.665	13.412	1.00	36.17
ATOM	4476	CD2	LEU	573	52.311	-6.042	13.032	1.00	32.13
ATOM	4477	C	LEU	573	51.117	-5.562	8.822	1.00	36.33

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ATOM	4478	O	LEU	573	50.477	-6.596	8.649	1.00	35.19
ATOM	4479	N	GLN	574	50.975	-4.502	8.038	1.00	37.66
ATOM	4481	CA	GLN	574	50.024	-4.514	6.936	1.00	41.78
ATOM	4482	CB	GLN	574	49.798	-3.103	6.413	1.00	43.82
ATOM	4483	CG	GLN	574	48.898	-2.273	7.264	1.00	45.42
ATOM	4484	CD	GLN	574	48.871	-0.850	6.801	1.00	49.56
ATOM	4485	OE1	GLN	574	49.456	-0.506	5.772	1.00	52.22
ATOM	4486	NE2	GLN	574	48.207	0.001	7.565	1.00	54.86
ATOM	4489	C	GLN	574	50.401	-5.427	5.783	1.00	42.89
ATOM	4490	O	GLN	574	49.532	-5.898	5.042	1.00	46.15
ATOM	4491	N	ALA	575	51.695	-5.646	5.599	1.00	42.39
ATOM	4493	CA	ALA	575	52.165	-6.516	4.532	1.00	40.19
ATOM	4494	CB	ALA	575	53.597	-6.165	4.170	1.00	40.68
ATOM	4495	C	ALA	575	52.088	-7.970	4.971	1.00	40.49
ATOM	4496	O	ALA	575	52.437	-8.867	4.210	1.00	43.34
ATOM	4497	N	ARG	576	51.630	-8.197	6.202	1.00	38.76
ATOM	4499	CA	ARG	576	51.538	-9.542	6.761	1.00	38.44
ATOM	4500	CB	ARG	576	52.600	-9.708	7.846	1.00	34.26
ATOM	4501	CG	ARG	576	53.991	-9.609	7.284	1.00	37.16
ATOM	4502	CD	ARG	576	55.052	-9.625	8.356	1.00	36.38
ATOM	4503	NE	ARG	576	56.384	-9.663	7.760	1.00	36.98
ATOM	4505	CZ	ARG	576	56.897	-8.714	6.983	1.00	38.62
ATOM	4506	NH1	ARG	576	56.204	-7.618	6.689	1.00	41.41
ATOM	4509	NH2	ARG	576	58.112	-8.863	6.491	1.00	37.48
ATOM	4512	C	ARG	576	50.165	-9.860	7.321	1.00	40.55
ATOM	4513	O	ARG	576	50.013	-10.746	8.169	1.00	43.20
ATOM	4514	N	ARG	577	49.156	-9.146	6.844	1.00	41.98
ATOM	4516	CA	ARG	577	47.794	-9.372	7.309	1.00	43.12
ATOM	4517	CB	ARG	577	46.896	-8.226	6.851	1.00	44.21
ATOM	4518	CG	ARG	577	47.206	-6.910	7.525	1.00	45.21
ATOM	4519	CD	ARG	577	46.402	-5.766	6.941	1.00	47.50
ATOM	4520	NE	ARG	577	46.172	-4.734	7.948	1.00	47.58
ATOM	4522	CZ	ARG	577	45.447	-3.641	7.752	1.00	47.63
ATOM	4523	NH1	ARG	577	44.882	-3.421	6.574	1.00	49.05
ATOM	4526	NH2	ARG	577	45.256	-2.789	8.747	1.00	49.88
ATOM	4529	C	ARG	577	47.241	-10.715	6.821	1.00	43.10
ATOM	4530	O	ARG	577	47.297	-11.015	5.627	1.00	43.86
ATOM	4531	N	GLN	594	53.448	-13.666	7.976	1.00	64.97
ATOM	4533	CA	GLN	594	52.231	-13.872	8.759	1.00	66.30
ATOM	4534	CB	GLN	594	51.419	-15.042	8.200	1.00	67.44
ATOM	4535	C	GLN	594	52.582	-14.116	10.224	1.00	66.02
ATOM	4536	O	GLN	594	53.162	-15.145	10.583	1.00	67.47
ATOM	4537	N	LEU	595	52.218	-13.151	11.058	1.00	62.86
ATOM	4539	CA	LEU	595	52.499	-13.187	12.480	1.00	59.77
ATOM	4540	CB	LEU	595	52.597	-11.751	12.987	1.00	59.35
ATOM	4541	CG	LEU	595	53.471	-10.905	12.051	1.00	61.70
ATOM	4542	CD1	LEU	595	53.307	-9.427	12.322	1.00	64.61
ATOM	4543	CD2	LEU	595	54.923	-11.324	12.175	1.00	62.38
ATOM	4544	C	LEU	595	51.482	-13.985	13.290	1.00	57.49
ATOM	4545	O	LEU	595	50.302	-14.026	12.951	1.00	56.36
ATOM	4546	N	SER	596	51.969	-14.647	14.338	1.00	55.62
ATOM	4548	CA	SER	596	51.134	-15.447	15.222	1.00	54.72
ATOM	4549	CB	SER	596	51.905	-16.669	15.721	1.00	55.13
ATOM	4550	OG	SER	596	52.871	-16.309	16.698	1.00	54.98

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ATOM	4552	C	SER	596	50.723	-14.597	16.415	1.00	54.73
ATOM	4553	O	SER	596	51.348	-13.579	16.704	1.00	53.29
ATOM	4554	N	SER	597	49.704	-15.051	17.137	1.00	55.09
ATOM	4556	CA	SER	597	49.215	-14.337	18.307	1.00	56.44
ATOM	4557	CB	SER	597	48.178	-15.185	19.044	1.00	59.14
ATOM	4558	OG	SER	597	47.455	-16.009	18.138	1.00	65.57
ATOM	4560	C	SER	597	50.387	-14.026	19.238	1.00	55.64
ATOM	4561	O	SER	597	50.430	-12.966	19.856	1.00	56.04
ATOM	4562	N	LYS	598	51.345	-14.948	19.315	1.00	54.91
ATOM	4564	CA	LYS	598	52.528	-14.773	20.161	1.00	54.25
ATOM	4565	CB	LYS	598	53.287	-16.096	20.311	1.00	54.23
ATOM	4566	CG	LYS	598	54.236	-16.138	21.494	1.00	55.12
ATOM	4567	CD	LYS	598	55.009	-17.448	21.523	1.00	59.41
ATOM	4568	CE	LYS	598	55.711	-17.679	22.858	1.00	58.10
ATOM	4569	NZ	LYS	598	54.750	-17.983	23.959	1.00	56.10
ATOM	4573	C	LYS	598	53.439	-13.716	19.536	1.00	52.32
ATOM	4574	O	LYS	598	53.986	-12.869	20.249	1.00	52.23
ATOM	4575	N	ASP	599	53.573	-13.768	18.208	1.00	47.57
ATOM	4577	CA	ASP	599	54.389	-12.818	17.466	1.00	45.47
ATOM	4578	CB	ASP	599	54.324	-13.101	15.959	1.00	49.05
ATOM	4579	CG	ASP	599	55.245	-14.238	15.525	1.00	54.16
ATOM	4580	OD1	ASP	599	56.242	-14.503	16.223	1.00	61.34
ATOM	4581	OD2	ASP	599	54.992	-14.863	14.471	1.00	55.80
ATOM	4582	C	ASP	599	53.933	-11.383	17.721	1.00	43.55
ATOM	4583	O	ASP	599	54.762	-10.491	17.895	1.00	44.34
ATOM	4584	N	LEU	600	52.622	-11.160	17.751	1.00	39.73
ATOM	4586	CA	LEU	600	52.104	-9.821	17.989	1.00	37.64
ATOM	4587	CB	LEU	600	50.597	-9.743	17.719	1.00	35.42
ATOM	4588	CG	LEU	600	50.075	-9.951	16.287	1.00	33.95
ATOM	4589	CD1	LEU	600	48.621	-9.552	16.262	1.00	36.59
ATOM	4590	CD2	LEU	600	50.841	-9.139	15.265	1.00	28.40
ATOM	4591	C	LEU	600	52.429	-9.347	19.402	1.00	38.24
ATOM	4592	O	LEU	600	52.817	-8.193	19.590	1.00	38.28
ATOM	4593	N	VAL	601	52.305	-10.235	20.391	1.00	38.77
ATOM	4595	CA	VAL	601	52.610	-9.855	21.772	1.00	38.87
ATOM	4596	CB	VAL	601	52.121	-10.906	22.812	1.00	38.03
ATOM	4597	CG1	VAL	601	52.150	-10.303	24.223	1.00	36.21
ATOM	4598	CG2	VAL	601	50.710	-11.332	22.504	1.00	39.07
ATOM	4599	C	VAL	601	54.123	-9.662	21.887	1.00	38.98
ATOM	4600	O	VAL	601	54.601	-8.757	22.580	1.00	39.93
ATOM	4601	N	SER	602	54.861	-10.488	21.155	1.00	37.35
ATOM	4603	CA	SER	602	56.311	-10.422	21.126	1.00	37.11
ATOM	4604	CB	SER	602	56.853	-11.469	20.154	1.00	39.38
ATOM	4605	OG	SER	602	58.265	-11.413	20.061	1.00	46.76
ATOM	4607	C	SER	602	56.695	-9.020	20.664	1.00	35.43
ATOM	4608	O	SER	602	57.493	-8.339	21.315	1.00	35.01
ATOM	4609	N	CYS	603	56.091	-8.586	19.561	1.00	33.42
ATOM	4611	CA	CYS	603	56.329	-7.254	19.015	1.00	32.18
ATOM	4612	CB	CYS	603	55.449	-7.035	17.790	1.00	32.38
ATOM	4613	SG	CYS	603	55.440	-5.365	17.123	0.50	35.11 PRT1
ATOM	4614	C	CYS	603	56.074	-6.167	20.059	1.00	31.20
ATOM	4615	O	CYS	603	56.862	-5.234	20.185	1.00	32.44
ATOM	4616	N	ALA	604	55.001	-6.321	20.828	1.00	29.74
ATOM	4618	CA	ALA	604	54.640	-5.363	21.872	1.00	32.26

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ATOM	4619	CB	ALA	604	53.232	-5.675	22.412	1.00	31.75
ATOM	4620	C	ALA	604	55.656	-5.365	23.019	1.00	33.71
ATOM	4621	O	ALA	604	55.933	-4.326	23.621	1.00	33.49
ATOM	4622	N	TYR	605	56.186	-6.544	23.326	1.00	35.56
ATOM	4624	CA	TYR	605	57.176	-6.709	24.388	1.00	35.49
ATOM	4625	CB	TYR	605	57.447	-8.206	24.617	1.00	36.12
ATOM	4626	CG	TYR	605	58.562	-8.495	25.591	1.00	34.75
ATOM	4627	CD1	TYR	605	58.415	-8.237	26.954	1.00	34.30
ATOM	4628	CE1	TYR	605	59.444	-8.499	27.853	1.00	36.26
ATOM	4629	CD2	TYR	605	59.773	-9.021	25.150	1.00	37.39
ATOM	4630	CE2	TYR	605	60.812	-9.288	26.040	1.00	37.81
ATOM	4631	CZ	TYR	605	60.641	-9.027	27.388	1.00	38.34
ATOM	4632	OH	TYR	605	61.662	-9.324	28.265	1.00	42.09
ATOM	4634	C	TYR	605	58.475	-5.972	24.027	1.00	34.98
ATOM	4635	O	TYR	605	58.981	-5.171	24.822	1.00	35.83
ATOM	4636	N	GLN	606	58.996	-6.247	22.828	1.00	33.99
ATOM	4638	CA	GLN	606	60.218	-5.620	22.315	1.00	33.60
ATOM	4639	CB	GLN	606	60.506	-6.111	20.894	1.00	31.37
ATOM	4640	CG	GLN	606	60.858	-7.584	20.786	1.00	32.05
ATOM	4641	CD	GLN	606	61.175	-8.015	19.354	1.00	30.33
ATOM	4642	OE1	GLN	606	62.145	-7.558	18.754	1.00	30.84
ATOM	4643	NE2	GLN	606	60.353	-8.895	18.810	1.00	33.75
ATOM	4646	C	GLN	606	60.123	-4.079	22.321	1.00	34.86
ATOM	4647	O	GLN	606	61.070	-3.390	22.702	1.00	37.54
ATOM	4648	N	VAL	607	58.975	-3.555	21.904	1.00	32.89
ATOM	4650	CA	VAL	607	58.748	-2.114	21.883	1.00	30.80
ATOM	4651	CB	VAL	607	57.426	-1.777	21.120	1.00	28.82
ATOM	4652	CG1	VAL	607	57.121	-0.299	21.191	1.00	25.36
ATOM	4653	CG2	VAL	607	57.541	-2.204	19.661	1.00	23.37
ATOM	4654	C	VAL	607	58.747	-1.532	23.312	1.00	30.48
ATOM	4655	O	VAL	607	59.359	-0.486	23.563	1.00	29.42
ATOM	4656	N	ALA	608	58.106	-2.225	24.255	1.00	30.07
ATOM	4658	CA	ALA	608	58.064	-1.761	25.646	1.00	30.14
ATOM	4659	CB	ALA	608	57.027	-2.548	26.452	1.00	28.49
ATOM	4660	C	ALA	608	59.455	-1.849	26.305	1.00	31.25
ATOM	4661	O	ALA	608	59.791	-1.054	27.198	1.00	28.90
ATOM	4662	N	ARG	609	60.257	-2.819	25.870	1.00	31.61
ATOM	4664	CA	ARG	609	61.608	-2.979	26.393	1.00	31.99
ATOM	4665	CB	ARG	609	62.253	-4.245	25.856	1.00	34.93
ATOM	4666	CG	ARG	609	61.606	-5.507	26.317	1.00	40.82
ATOM	4667	CD	ARG	609	62.633	-6.606	26.397	1.00	42.68
ATOM	4668	NE	ARG	609	63.275	-6.621	27.705	1.00	43.85
ATOM	4670	CZ	ARG	609	64.332	-7.364	28.019	1.00	44.73
ATOM	4671	NH1	ARG	609	64.889	-8.162	27.108	1.00	41.40
ATOM	4674	NH2	ARG	609	64.803	-7.341	29.260	1.00	44.85
ATOM	4677	C	ARG	609	62.459	-1.796	25.966	1.00	33.70
ATOM	4678	O	ARG	609	63.130	-1.174	26.793	1.00	35.94
ATOM	4679	N	GLY	610	62.459	-1.511	24.663	1.00	31.22
ATOM	4681	CA	GLY	610	63.232	-0.391	24.157	1.00	27.21
ATOM	4682	C	GLY	610	62.819	0.875	24.865	1.00	25.81
ATOM	4683	O	GLY	610	63.665	1.652	25.300	1.00	26.21
ATOM	4684	N	MET	611	61.511	1.056	25.015	1.00	27.12
ATOM	4686	CA	MET	611	60.969	2.222	25.695	1.00	28.82
ATOM	4687	CB	MET	611	59.457	2.288	25.524	1.00	29.29

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ATOM	4688	CG	MET	611	59.004	2.706	24.135	1.00	31.07
ATOM	4689	SD	MET	611	59.732	4.286	23.617	1.00	28.38
ATOM	4690	CE	MET	611	59.155	5.431	24.922	1.00	28.34
ATOM	4691	C	MET	611	61.341	2.261	27.178	1.00	30.34
ATOM	4692	O	MET	611	61.596	3.334	27.730	1.00	31.73
ATOM	4693	N	GLU	612	61.347	1.109	27.837	1.00	32.72
ATOM	4695	CA	GLU	612	61.723	1.057	29.253	1.00	35.46
ATOM	4696	CB	GLU	612	61.603	-0.370	29.792	1.00	34.70
ATOM	4697	CG	GLU	612	62.029	-0.516	31.237	1.00	32.31
ATOM	4698	CD	GLU	612	62.135	-1.968	31.688	1.00	33.14
ATOM	4699	OE1	GLU	612	62.546	-2.834	30.883	1.00	30.79
ATOM	4700	OE2	GLU	612	61.826	-2.240	32.867	1.00	36.13
ATOM	4701	C	GLU	612	63.178	1.544	29.353	1.00	36.43
ATOM	4702	O	GLU	612	63.534	2.319	30.261	1.00	35.38
ATOM	4703	N	TYR	613	63.999	1.107	28.391	1.00	35.47
ATOM	4705	CA	TYR	613	65.403	1.507	28.334	1.00	33.16
ATOM	4706	CB	TYR	613	66.156	0.743	27.241	1.00	31.33
ATOM	4707	CG	TYR	613	67.612	1.146	27.132	1.00	33.03
ATOM	4708	CD1	TYR	613	68.584	0.544	27.931	1.00	36.69
ATOM	4709	CE1	TYR	613	69.930	0.927	27.851	1.00	36.82
ATOM	4710	CD2	TYR	613	68.021	2.148	26.247	1.00	33.49
ATOM	4711	CE2	TYR	613	69.352	2.540	26.157	1.00	34.73
ATOM	4712	CZ	TYR	613	70.307	1.927	26.963	1.00	37.07
ATOM	4713	OH	TYR	613	71.632	2.318	26.896	1.00	36.77
ATOM	4715	C	TYR	613	65.539	3.005	28.088	1.00	31.82
ATOM	4716	O	TYR	613	66.256	3.682	28.814	1.00	34.76
ATOM	4717	N	LEU	614	64.836	3.536	27.090	1.00	28.44
ATOM	4719	CA	LEU	614	64.931	4.956	26.793	1.00	25.67
ATOM	4720	CB	LEU	614	64.089	5.319	25.569	1.00	24.75
ATOM	4721	CG	LEU	614	64.545	4.778	24.208	1.00	23.73
ATOM	4722	CD1	LEU	614	63.594	5.257	23.125	1.00	20.54
ATOM	4723	CD2	LEU	614	65.983	5.213	23.894	1.00	23.21
ATOM	4724	C	LEU	614	64.499	5.761	28.001	1.00	28.30
ATOM	4725	O	LEU	614	65.110	6.770	28.345	1.00	27.09
ATOM	4726	N	ALA	615	63.470	5.272	28.683	1.00	32.73
ATOM	4728	CA	ALA	615	62.955	5.945	29.871	1.00	34.10
ATOM	4729	CB	ALA	615	61.625	5.314	30.314	1.00	33.68
ATOM	4730	C	ALA	615	63.986	5.913	31.007	1.00	33.84
ATOM	4731	O	ALA	615	64.112	6.885	31.753	1.00	34.95
ATOM	4732	N	SER	616	64.722	4.809	31.134	1.00	32.69
ATOM	4734	CA	SER	616	65.738	4.703	32.175	1.00	33.50
ATOM	4735	CB	SER	616	66.287	3.277	32.285	1.00	28.27
ATOM	4736	OG	SER	616	67.076	2.935	31.165	1.00	25.54
ATOM	4738	C	SER	616	66.870	5.678	31.865	1.00	35.43
ATOM	4739	O	SER	616	67.637	6.061	32.755	1.00	37.32
ATOM	4740	N	LYS	617	66.971	6.060	30.592	1.00	34.80
ATOM	4742	CA	LYS	617	67.975	7.010	30.143	1.00	33.01
ATOM	4743	CB	LYS	617	68.508	6.620	28.776	1.00	33.18
ATOM	4744	CG	LYS	617	69.224	5.302	28.797	1.00	35.64
ATOM	4745	CD	LYS	617	70.423	5.380	29.710	1.00	40.31
ATOM	4746	CE	LYS	617	71.075	4.025	29.863	1.00	43.03
ATOM	4747	NZ	LYS	617	72.426	4.152	30.449	1.00	45.54
ATOM	4751	C	LYS	617	67.360	8.397	30.102	1.00	32.87
ATOM	4752	O	LYS	617	67.892	9.308	29.470	1.00	34.06

ATOM	4753	N	LYS	618	66.221	8.542	30.772	1.00	33.53
ATOM	4755	CA	LYS	618	65.500	9.808	30.872	1.00	33.28
ATOM	4756	CB	LYS	618	66.384	10.842	31.558	1.00	37.22
ATOM	4757	CG	LYS	618	66.968	10.367	32.869	1.00	43.11
ATOM	4758	CD	LYS	618	65.927	10.278	33.957	1.00	49.82
ATOM	4759	CE	LYS	618	66.520	9.636	35.199	1.00	55.20
ATOM	4760	NZ	LYS	618	65.669	9.853	36.415	1.00	61.31
ATOM	4764	C	LYS	618	65.012	10.359	29.542	1.00	31.57
ATOM	4765	O	LYS	618	64.651	11.530	29.455	1.00	31.10
ATOM	4766	N	CYS	619	64.953	9.506	28.524	1.00	31.04
ATOM	4768	CA	CYS	619	64.519	9.922	27.196	1.00	29.21
ATOM	4769	CB	CYS	619	65.213	9.065	26.125	1.00	28.55
ATOM	4770	SG	CYS	619	64.782	9.400	24.392	1.00	26.31
ATOM	4771	C	CYS	619	62.999	9.849	27.051	1.00	30.91
ATOM	4772	O	CYS	619	62.376	8.827	27.364	1.00	31.18
ATOM	4773	N	ILE	620	62.411	10.967	26.632	1.00	29.48
ATOM	4775	CA	ILE	620	60.981	11.073	26.416	1.00	29.34
ATOM	4776	CB	ILE	620	60.402	12.344	27.060	1.00	28.12
ATOM	4777	CG2	ILE	620	58.944	12.535	26.645	1.00	28.76
ATOM	4778	CG1	ILE	620	60.521	12.267	28.581	1.00	28.36
ATOM	4779	CD1	ILE	620	60.062	13.522	29.270	1.00	25.55
ATOM	4780	C	ILE	620	60.852	11.188	24.908	1.00	30.97
ATOM	4781	O	ILE	620	61.254	12.193	24.336	1.00	33.88
ATOM	4782	N	HIS	621	60.307	10.147	24.284	1.00	31.55
ATOM	4784	CA	HIS	621	60.148	10.080	22.831	1.00	31.85
ATOM	4785	CB	HIS	621	59.721	8.668	22.425	1.00	28.27
ATOM	4786	CG	HIS	621	59.913	8.373	20.979	1.00	24.68
ATOM	4787	CD2	HIS	621	60.608	7.383	20.356	1.00	24.39
ATOM	4788	ND1	HIS	621	59.354	9.130	19.973	1.00	25.87
ATOM	4790	CE1	HIS	621	59.691	8.623	18.798	1.00	27.65
ATOM	4791	NE2	HIS	621	60.444	7.571	19.007	1.00	25.80
ATOM	4793	C	HIS	621	59.187	11.096	22.224	1.00	34.38
ATOM	4794	O	HIS	621	59.387	11.539	21.104	1.00	38.74
ATOM	4795	N	ARG	622	58.080	11.374	22.898	1.00	37.17
ATOM	4797	CA	ARG	622	57.093	12.346	22.425	1.00	37.27
ATOM	4798	CB	ARG	622	57.718	13.746	22.298	1.00	38.63
ATOM	4799	CG	ARG	622	58.261	14.271	23.601	1.00	40.47
ATOM	4800	CD	ARG	622	58.661	15.739	23.530	1.00	44.76
ATOM	4801	NE	ARG	622	59.129	16.174	24.842	1.00	52.09
ATOM	4803	CZ	ARG	622	60.299	15.821	25.375	1.00	56.86
ATOM	4804	NH1	ARG	622	61.132	15.041	24.699	1.00	61.20
ATOM	4807	NH2	ARG	622	60.606	16.167	26.624	1.00	58.19
ATOM	4810	C	ARG	622	56.324	11.994	21.151	1.00	37.23
ATOM	4811	O	ARG	622	55.300	12.614	20.867	1.00	38.45
ATOM	4812	N	ASP	623	56.805	11.035	20.364	1.00	36.55
ATOM	4814	CA	ASP	623	56.075	10.652	19.160	1.00	36.52
ATOM	4815	CB	ASP	623	56.581	11.403	17.910	1.00	39.68
ATOM	4816	CG	ASP	623	55.635	11.247	16.687	1.00	48.75
ATOM	4817	OD1	ASP	623	56.077	11.491	15.538	1.00	49.98
ATOM	4818	OD2	ASP	623	54.445	10.879	16.872	1.00	49.65
ATOM	4819	C	ASP	623	56.126	9.143	18.967	1.00	33.37
ATOM	4820	O	ASP	623	56.325	8.650	17.864	1.00	31.77
ATOM	4821	N	LEU	624	55.999	8.404	20.059	1.00	30.45
ATOM	4823	CA	LEU	624	56.014	6.954	19.950	1.00	30.77

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ATOM	4824	CB	LEU	624	55.983	6.307	21.342	1.00	27.43
ATOM	4825	CG	LEU	624	55.949	4.778	21.441	1.00	28.69
ATOM	4826	CD1	LEU	624	57.139	4.132	20.731	1.00	24.75
ATOM	4827	CD2	LEU	624	55.927	4.389	22.894	1.00	27.39
ATOM	4828	C	LEU	624	54.803	6.532	19.109	1.00	31.22
ATOM	4829	O	LEU	624	53.680	6.952	19.380	1.00	33.44
ATOM	4830	N	ALA	625	55.053	5.763	18.054	1.00	28.85
ATOM	4832	CA	ALA	625	54.009	5.286	17.159	1.00	26.93
ATOM	4833	CB	ALA	625	53.559	6.400	16.227	1.00	25.03
ATOM	4834	C	ALA	625	54.642	4.162	16.356	1.00	28.44
ATOM	4835	O	ALA	625	55.863	4.065	16.317	1.00	31.32
ATOM	4836	N	ALA	626	53.828	3.329	15.705	1.00	29.14
ATOM	4838	CA	ALA	626	54.344	2.205	14.905	1.00	28.42
ATOM	4839	CB	ALA	626	53.192	1.357	14.353	1.00	27.37
ATOM	4840	C	ALA	626	55.231	2.698	13.771	1.00	26.38
ATOM	4841	O	ALA	626	56.195	2.041	13.395	1.00	26.12
ATOM	4842	N	ARG	627	54.890	3.861	13.230	1.00	27.16
ATOM	4844	CA	ARG	627	55.669	4.474	12.158	1.00	28.44
ATOM	4845	CB	ARG	627	55.022	5.794	11.733	1.00	28.19
ATOM	4846	CG	ARG	627	54.889	6.793	12.867	1.00	30.34
ATOM	4847	CD	ARG	627	54.456	8.155	12.361	1.00	34.08
ATOM	4848	NE	ARG	627	54.081	9.024	13.471	1.00	35.58
ATOM	4850	CZ	ARG	627	52.849	9.123	13.950	1.00	35.55
ATOM	4851	NH1	ARG	627	51.860	8.422	13.420	1.00	35.67
ATOM	4854	NH2	ARG	627	52.618	9.898	14.993	1.00	40.81
ATOM	4857	C	ARG	627	57.108	4.733	12.630	1.00	28.06
ATOM	4858	O	ARG	627	58.044	4.737	11.825	1.00	29.80
ATOM	4859	N	ASN	628	57.272	4.935	13.940	1.00	28.50
ATOM	4861	CA	ASN	628	58.582	5.195	14.544	1.00	26.14
ATOM	4862	CB	ASN	628	58.494	6.340	15.551	1.00	23.55
ATOM	4863	CG	ASN	628	58.319	7.681	14.874	1.00	27.48
ATOM	4864	OD1	ASN	628	58.874	7.919	13.800	1.00	34.12
ATOM	4865	ND2	ASN	628	57.543	8.556	15.479	1.00	23.21
ATOM	4868	C	ASN	628	59.263	3.965	15.153	1.00	26.76
ATOM	4869	O	ASN	628	60.202	4.078	15.948	1.00	26.90
ATOM	4870	N	VAL	629	58.774	2.794	14.767	1.00	27.02
ATOM	4872	CA	VAL	629	59.344	1.523	15.186	1.00	27.81
ATOM	4873	CB	VAL	629	58.298	0.622	15.864	1.00	26.83
ATOM	4874	CG1	VAL	629	58.876	-0.766	16.115	1.00	20.74
ATOM	4875	CG2	VAL	629	57.836	1.259	17.165	1.00	22.49
ATOM	4876	C	VAL	629	59.781	0.895	13.861	1.00	28.61
ATOM	4877	O	VAL	629	58.983	0.809	12.924	1.00	28.76
ATOM	4878	N	LEU	630	61.059	0.557	13.746	1.00	30.35
ATOM	4880	CA	LEU	630	61.576	-0.033	12.514	1.00	32.42
ATOM	4881	CB	LEU	630	62.824	0.725	12.040	1.00	32.28
ATOM	4882	CG	LEU	630	62.697	2.249	11.880	1.00	27.75
ATOM	4883	CD1	LEU	630	64.019	2.860	11.469	1.00	24.71
ATOM	4884	CD2	LEU	630	61.611	2.582	10.872	1.00	27.70
ATOM	4885	C	LEU	630	61.895	-1.488	12.799	1.00	32.89
ATOM	4886	O	LEU	630	62.167	-1.838	13.943	1.00	32.32
ATOM	4887	N	VAL	631	61.831	-2.336	11.774	1.00	34.81
ATOM	4889	CA	VAL	631	62.087	-3.772	11.943	1.00	33.87
ATOM	4890	CB	VAL	631	60.818	-4.616	11.597	1.00	31.60
ATOM	4891	CG1	VAL	631	60.929	-6.004	12.197	1.00	30.84

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ATOM	4892	CG2	VAL	631	59.545	-3.916	12.089	1.00	25.53
ATOM	4893	C	VAL	631	63.286	-4.256	11.109	1.00	34.95
ATOM	4894	O	VAL	631	63.365	-4.009	9.892	1.00	37.01
ATOM	4895	N	THR	632	64.215	-4.942	11.770	1.00	35.08
ATOM	4897	CA	THR	632	65.418	-5.444	11.104	1.00	35.96
ATOM	4898	CB	THR	632	66.541	-5.711	12.116	1.00	34.29
ATOM	4899	OG1	THR	632	66.187	-6.818	12.953	1.00	32.35
ATOM	4901	CG2	THR	632	66.750	-4.488	12.985	1.00	33.42
ATOM	4902	C	THR	632	65.162	-6.712	10.300	1.00	39.32
ATOM	4903	O	THR	632	64.078	-7.302	10.382	1.00	41.24
ATOM	4904	N	GLU	633	66.153	-7.123	9.511	1.00	42.32
ATOM	4906	CA	GLU	633	66.030	-8.335	8.703	1.00	44.34
ATOM	4907	CB	GLU	633	67.314	-8.609	7.912	1.00	46.06
ATOM	4908	CG	GLU	633	67.205	-9.767	6.898	1.00	49.87
ATOM	4909	CD	GLU	633	66.380	-9.445	5.629	1.00	53.04
ATOM	4910	OE1	GLU	633	65.637	-8.430	5.570	1.00	51.31
ATOM	4911	OE2	GLU	633	66.479	-10.226	4.667	1.00	55.48
ATOM	4912	C	GLU	633	65.708	-9.526	9.600	1.00	44.58
ATOM	4913	O	GLU	633	64.974	-10.423	9.207	1.00	46.56
ATOM	4914	N	ASP	634	66.201	-9.493	10.833	1.00	44.12
ATOM	4916	CA	ASP	634	65.961	-10.583	11.759	1.00	44.23
ATOM	4917	CB	ASP	634	67.221	-10.867	12.580	1.00	50.17
ATOM	4918	CG	ASP	634	68.443	-11.181	11.697	1.00	56.79
ATOM	4919	OD1	ASP	634	68.363	-12.113	10.857	1.00	59.62
ATOM	4920	OD2	ASP	634	69.482	-10.490	11.837	1.00	58.62
ATOM	4921	C	ASP	634	64.756	-10.331	12.644	1.00	43.26
ATOM	4922	O	ASP	634	64.652	-10.879	13.733	1.00	43.58
ATOM	4923	N	ASN	635	63.858	-9.475	12.166	1.00	43.97
ATOM	4925	CA	ASN	635	62.612	-9.126	12.847	1.00	43.66
ATOM	4926	CB	ASN	635	61.698	-10.355	12.930	1.00	46.94
ATOM	4927	CG	ASN	635	61.413	-10.958	11.572	1.00	48.19
ATOM	4928	OD1	ASN	635	60.831	-10.314	10.702	1.00	51.42
ATOM	4929	ND2	ASN	635	61.832	-12.198	11.380	1.00	49.44
ATOM	4932	C	ASN	635	62.694	-8.463	14.216	1.00	43.03
ATOM	4933	O	ASN	635	61.774	-8.596	15.031	1.00	43.03
ATOM	4934	N	VAL	636	63.763	-7.712	14.467	1.00	42.69
ATOM	4936	CA	VAL	636	63.915	-7.034	15.756	1.00	38.30
ATOM	4937	CB	VAL	636	65.406	-6.861	16.134	1.00	37.92
ATOM	4938	CG1	VAL	636	65.555	-6.040	17.421	1.00	37.14
ATOM	4939	CG2	VAL	636	66.052	-8.226	16.306	1.00	37.55
ATOM	4940	C	VAL	636	63.251	-5.673	15.688	1.00	35.75
ATOM	4941	O	VAL	636	63.486	-4.926	14.746	1.00	36.28
ATOM	4942	N	MET	637	62.355	-5.396	16.628	1.00	34.73
ATOM	4944	CA	MET	637	61.672	-4.103	16.680	1.00	33.22
ATOM	4945	CB	MET	637	60.456	-4.152	17.608	1.00	34.83
ATOM	4946	CG	MET	637	59.364	-5.148	17.231	1.00	34.41
ATOM	4947	SD	MET	637	58.661	-4.926	15.589	1.00	33.19
ATOM	4948	CE	MET	637	58.869	-6.584	14.913	1.00	29.73
ATOM	4949	C	MET	637	62.677	-3.107	17.250	1.00	33.75
ATOM	4950	O	MET	637	63.281	-3.357	18.308	1.00	31.79
ATOM	4951	N	LYS	638	62.839	-1.980	16.558	1.00	31.83
ATOM	4953	CA	LYS	638	63.774	-0.939	16.965	1.00	28.17
ATOM	4954	CB	LYS	638	64.986	-0.930	16.038	1.00	24.98
ATOM	4955	CG	LYS	638	66.006	-1.967	16.400	1.00	23.17

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ATOM	4956	CD	LYS	638	67.193	-1.916	15.470	1.00	25.04
ATOM	4957	CE	LYS	638	68.212	-2.969	15.847	1.00	24.79
ATOM	4958	NZ	LYS	638	68.747	-2.765	17.220	1.00	24.91
ATOM	4962	C	LYS	638	63.165	0.445	16.986	1.00	26.04
ATOM	4963	O	LYS	638	62.803	0.958	15.936	1.00	24.44
ATOM	4964	N	ILE	639	63.052	1.031	18.181	1.00	25.14
ATOM	4966	CA	ILE	639	62.508	2.376	18.351	1.00	25.68
ATOM	4967	CB	ILE	639	62.589	2.863	19.839	1.00	27.40
ATOM	4968	CG2	ILE	639	61.875	4.189	19.984	1.00	18.94
ATOM	4969	CG1	ILE	639	62.019	1.827	20.826	1.00	26.05
ATOM	4970	CD1	ILE	639	60.517	1.667	20.792	1.00	25.07
ATOM	4971	C	ILE	639	63.387	3.338	17.543	1.00	25.82
ATOM	4972	O	ILE	639	64.619	3.283	17.642	1.00	25.76
ATOM	4973	N	ALA	640	62.758	4.231	16.783	1.00	25.92
ATOM	4975	CA	ALA	640	63.477	5.218	15.976	1.00	26.12
ATOM	4976	CB	ALA	640	63.222	4.964	14.506	1.00	26.54
ATOM	4977	C	ALA	640	63.042	6.643	16.344	1.00	26.33
ATOM	4978	O	ALA	640	61.996	6.828	16.974	1.00	26.20
ATOM	4979	N	ASP	641	63.863	7.637	15.993	1.00	26.59
ATOM	4981	CA	ASP	641	63.545	9.052	16.245	1.00	28.09
ATOM	4982	CB	ASP	641	62.217	9.443	15.593	1.00	31.43
ATOM	4983	CG	ASP	641	62.346	9.762	14.107	1.00	36.81
ATOM	4984	OD1	ASP	641	63.409	9.478	13.500	1.00	40.24
ATOM	4985	OD2	ASP	641	61.356	10.299	13.548	1.00	40.49
ATOM	4986	C	ASP	641	63.455	9.442	17.700	1.00	28.40
ATOM	4987	O	ASP	641	62.825	10.446	18.041	1.00	29.30
ATOM	4988	N	PHE	642	64.080	8.658	18.564	1.00	30.27
ATOM	4990	CA	PHE	642	64.044	8.943	19.992	1.00	30.97
ATOM	4991	CB	PHE	642	64.327	7.664	20.787	1.00	24.64
ATOM	4992	CG	PHE	642	65.673	7.063	20.505	1.00	20.96
ATOM	4993	CD1	PHE	642	66.812	7.539	21.163	1.00	16.89
ATOM	4994	CD2	PHE	642	65.806	6.026	19.576	1.00	16.23
ATOM	4995	CE1	PHE	642	68.072	6.990	20.900	1.00	18.35
ATOM	4996	CE2	PHE	642	67.051	5.471	19.305	1.00	18.76
ATOM	4997	CZ	PHE	642	68.195	5.954	19.970	1.00	17.91
ATOM	4998	C	PHE	642	65.024	10.045	20.414	1.00	34.53
ATOM	4999	O	PHE	642	64.990	10.503	21.563	1.00	35.23
ATOM	5000	N	GLY	643	65.910	10.433	19.500	1.00	36.40
ATOM	5002	CA	GLY	643	66.888	11.455	19.799	1.00	38.28
ATOM	5003	C	GLY	643	66.634	12.768	19.093	1.00	41.44
ATOM	5004	O	GLY	643	67.482	13.652	19.132	1.00	44.10
ATOM	5005	N	LEU	644	65.461	12.921	18.484	1.00	45.44
ATOM	5007	CA	LEU	644	65.131	14.144	17.748	1.00	49.14
ATOM	5008	CB	LEU	644	63.832	13.975	16.969	1.00	46.26
ATOM	5009	CG	LEU	644	63.823	12.967	15.836	1.00	42.90
ATOM	5010	CD1	LEU	644	62.527	13.134	15.070	1.00	42.68
ATOM	5011	CD2	LEU	644	65.004	13.228	14.934	1.00	45.15
ATOM	5012	C	LEU	644	65.027	15.396	18.605	1.00	53.90
ATOM	5013	O	LEU	644	64.488	15.356	19.715	1.00	56.54
ATOM	5014	N	ALA	645	65.534	16.505	18.068	1.00	57.59
ATOM	5016	CA	ALA	645	65.505	17.794	18.759	1.00	60.15
ATOM	5017	CB	ALA	645	66.539	18.741	18.156	1.00	59.55
ATOM	5018	C	ALA	645	64.112	18.407	18.667	1.00	61.90
ATOM	5019	O	ALA	645	63.393	18.500	19.663	1.00	63.83

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ATOM	5020	N	ASP	652	52.090	22.191	14.865	1.00	89.91
ATOM	5022	CA	ASP	652	50.913	22.199	14.007	1.00	89.75
ATOM	5023	CB	ASP	652	51.314	22.428	12.537	1.00	88.08
ATOM	5024	CG	ASP	652	50.109	22.557	11.607	1.00	87.09
ATOM	5025	OD1	ASP	652	49.028	22.996	12.052	1.00	86.85
ATOM	5026	OD2	ASP	652	50.252	22.222	10.411	1.00	86.69
ATOM	5027	C	ASP	652	50.145	20.890	14.156	1.00	89.98
ATOM	5028	O	ASP	652	50.434	19.899	13.483	1.00	90.19
ATOM	5029	N	TYR	653	49.145	20.905	15.027	1.00	90.26
ATOM	5031	CA	TYR	653	48.318	19.730	15.277	1.00	90.78
ATOM	5032	CB	TYR	653	47.272	20.048	16.344	1.00	91.65
ATOM	5033	CG	TYR	653	47.804	20.185	17.755	1.00	93.43
ATOM	5034	CD1	TYR	653	47.017	20.757	18.752	1.00	94.60
ATOM	5035	CE1	TYR	653	47.477	20.885	20.058	1.00	95.35
ATOM	5036	CD2	TYR	653	49.083	19.738	18.101	1.00	93.46
ATOM	5037	CE2	TYR	653	49.558	19.860	19.406	1.00	94.36
ATOM	5038	CZ	TYR	653	48.748	20.435	20.378	1.00	95.26
ATOM	5039	OH	TYR	653	49.220	20.554	21.669	1.00	95.00
ATOM	5041	C	TYR	653	47.602	19.231	14.021	1.00	90.47
ATOM	5042	O	TYR	653	47.045	18.131	14.012	1.00	91.33
ATOM	5043	N	TYR	654	47.632	20.031	12.962	1.00	89.21
ATOM	5045	CA	TYR	654	46.954	19.673	11.727	1.00	89.09
ATOM	5046	CB	TYR	654	46.205	20.893	11.188	1.00	88.23
ATOM	5047	CG	TYR	654	45.275	21.499	12.209	1.00	87.65
ATOM	5048	CD1	TYR	654	45.776	22.140	13.343	1.00	86.76
ATOM	5049	CE1	TYR	654	44.929	22.655	14.312	1.00	87.17
ATOM	5050	CD2	TYR	654	43.895	21.396	12.067	1.00	88.61
ATOM	5051	CE2	TYR	654	43.032	21.912	13.033	1.00	89.32
ATOM	5052	CZ	TYR	654	43.557	22.538	14.153	1.00	88.66
ATOM	5053	OH	TYR	654	42.710	23.034	15.117	1.00	89.39
ATOM	5055	C	TYR	654	47.857	19.080	10.651	1.00	89.49
ATOM	5056	O	TYR	654	47.396	18.772	9.552	1.00	88.37
ATOM	5057	N	LYS	655	49.139	18.919	10.959	1.00	90.80
ATOM	5059	CA	LYS	655	50.056	18.356	9.982	1.00	93.18
ATOM	5060	CB	LYS	655	51.508	18.713	10.311	1.00	95.66
ATOM	5061	CG	LYS	655	52.504	18.133	9.315	1.00	99.82
ATOM	5062	CD	LYS	655	53.932	18.585	9.562	1.00	103.58
ATOM	5063	CE	LYS	655	54.898	17.833	8.637	1.00	106.15
ATOM	5064	NZ	LYS	655	56.325	18.246	8.821	1.00	108.43
ATOM	5068	C	LYS	655	49.884	16.847	9.935	1.00	93.56
ATOM	5069	O	LYS	655	49.904	16.182	10.972	1.00	93.72
ATOM	5070	N	LYS	656	49.670	16.320	8.735	1.00	94.19
ATOM	5072	CA	LYS	656	49.500	14.886	8.545	1.00	94.84
ATOM	5073	CB	LYS	656	48.628	14.620	7.320	1.00	94.64
ATOM	5074	CG	LYS	656	47.155	14.874	7.542	1.00	95.54
ATOM	5075	CD	LYS	656	46.402	14.709	6.241	1.00	99.56
ATOM	5076	CE	LYS	656	44.926	14.449	6.473	1.00	101.77
ATOM	5077	NZ	LYS	656	44.202	14.327	5.173	1.00	103.77
ATOM	5081	C	LYS	656	50.859	14.225	8.368	1.00	95.18
ATOM	5082	O	LYS	656	51.823	14.878	7.956	1.00	95.74
ATOM	5083	N	GLY	660	48.651	9.665	5.782	1.00	58.76
ATOM	5085	CA	GLY	660	47.932	10.910	6.012	1.00	56.04
ATOM	5086	C	GLY	660	47.241	10.937	7.364	1.00	53.90
ATOM	5087	O	GLY	660	46.183	11.552	7.525	1.00	53.92

ATOM	5088	N	ARG	661	47.838	10.243	8.328	1.00	51.87
ATOM	5090	CA	ARG	661	47.297	10.177	9.679	1.00	48.23
ATOM	5091	CB	ARG	661	47.755	8.891	10.377	1.00	49.74
ATOM	5092	CG	ARG	661	47.506	7.620	9.566	1.00	47.59
ATOM	5093	CD	ARG	661	47.561	6.390	10.446	1.00	51.85
ATOM	5094	NE	ARG	661	47.584	5.155	9.663	1.00	52.94
ATOM	5096	CZ	ARG	661	48.035	3.988	10.117	1.00	52.19
ATOM	5097	NH1	ARG	661	48.503	3.884	11.356	1.00	52.10
ATOM	5100	NH2	ARG	661	48.036	2.926	9.327	1.00	54.43
ATOM	5103	C	ARG	661	47.722	11.401	10.483	1.00	43.67
ATOM	5104	O	ARG	661	48.658	12.103	10.104	1.00	41.45
ATOM	5105	N	LEU	662	47.019	11.656	11.579	1.00	40.27
ATOM	5107	CA	LEU	662	47.310	12.799	12.437	1.00	37.15
ATOM	5108	CB	LEU	662	46.021	13.533	12.783	1.00	37.39
ATOM	5109	CG	LEU	662	45.301	14.149	11.588	1.00	37.67
ATOM	5110	CD1	LEU	662	43.852	14.428	11.937	1.00	35.38
ATOM	5111	CD2	LEU	662	46.041	15.407	11.163	1.00	39.79
ATOM	5112	C	LEU	662	47.973	12.330	13.716	1.00	34.68
ATOM	5113	O	LEU	662	47.327	11.718	14.568	1.00	33.33
ATOM	5114	N	PRO	663	49.260	12.655	13.892	1.00	34.11
ATOM	5115	CD	PRO	663	50.086	13.389	12.924	1.00	33.67
ATOM	5116	CA	PRO	663	50.052	12.281	15.068	1.00	33.55
ATOM	5117	CB	PRO	663	51.367	13.003	14.833	1.00	32.99
ATOM	5118	CG	PRO	663	51.479	12.966	13.328	1.00	36.09
ATOM	5119	C	PRO	663	49.412	12.665	16.399	1.00	33.55
ATOM	5120	O	PRO	663	49.683	12.036	17.426	1.00	34.11
ATOM	5121	N	VAL	664	48.566	13.697	16.387	1.00	32.63
ATOM	5123	CA	VAL	664	47.874	14.092	17.613	1.00	32.24
ATOM	5124	CB	VAL	664	46.953	15.327	17.396	1.00	33.24
ATOM	5125	CG1	VAL	664	47.779	16.583	17.252	1.00	35.01
ATOM	5126	CG2	VAL	664	46.089	15.154	16.155	1.00	35.44
ATOM	5127	C	VAL	664	47.072	12.896	18.150	1.00	31.08
ATOM	5128	O	VAL	664	46.866	12.760	19.360	1.00	31.49
ATOM	5129	N	LYS	665	46.710	11.978	17.255	1.00	29.75
ATOM	5131	CA	LYS	665	45.956	10.788	17.638	1.00	28.83
ATOM	5132	CB	LYS	665	45.411	10.083	16.397	1.00	29.52
ATOM	5133	CG	LYS	665	44.242	10.835	15.797	1.00	27.21
ATOM	5134	CD	LYS	665	43.905	10.431	14.397	1.00	27.25
ATOM	5135	CE	LYS	665	42.684	11.228	13.931	1.00	28.63
ATOM	5136	NZ	LYS	665	42.266	10.902	12.545	1.00	25.33
ATOM	5140	C	LYS	665	46.718	9.830	18.537	1.00	29.03
ATOM	5141	O	LYS	665	46.152	8.869	19.046	1.00	28.37
ATOM	5142	N	TRP	666	47.994	10.123	18.765	1.00	30.40
ATOM	5144	CA	TRP	666	48.825	9.296	19.628	1.00	31.10
ATOM	5145	CB	TRP	666	50.123	8.906	18.917	1.00	29.53
ATOM	5146	CG	TRP	666	49.946	7.781	17.966	1.00	27.03
ATOM	5147	CD2	TRP	666	49.407	7.853	16.638	1.00	25.06
ATOM	5148	CE2	TRP	666	49.418	6.546	16.116	1.00	23.83
ATOM	5149	CE3	TRP	666	48.924	8.899	15.835	1.00	26.08
ATOM	5150	CD1	TRP	666	50.257	6.475	18.186	1.00	20.75
ATOM	5151	NE1	TRP	666	49.937	5.729	17.086	1.00	24.92
ATOM	5153	CZ2	TRP	666	48.962	6.245	14.832	1.00	23.95
ATOM	5154	CZ3	TRP	666	48.466	8.604	14.548	1.00	29.09
ATOM	5155	CH2	TRP	666	48.491	7.282	14.060	1.00	29.22

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ATOM	5156	C	TRP	666	49.174	10.049	20.896	1.00	33.20
ATOM	5157	O	TRP	666	49.701	9.469	21.849	1.00	34.39
ATOM	5158	N	MET	667	48.862	11.340	20.910	1.00	34.82
ATOM	5160	CA	MET	667	49.169	12.175	22.056	1.00	36.31
ATOM	5161	CB	MET	667	49.205	13.645	21.651	1.00	40.08
ATOM	5162	CG	MET	667	50.475	14.047	20.931	1.00	42.41
ATOM	5163	SD	MET	667	50.555	15.818	20.713	1.00	51.31
ATOM	5164	CE	MET	667	50.957	15.928	18.949	1.00	45.44
ATOM	5165	C	MET	667	48.299	12.003	23.287	1.00	37.81
ATOM	5166	O	MET	667	47.081	11.871	23.195	1.00	38.91
ATOM	5167	N	ALA	668	48.958	11.964	24.442	1.00	36.47
ATOM	5169	CA	ALA	668	48.286	11.846	25.718	1.00	37.06
ATOM	5170	CB	ALA	668	49.308	11.654	26.835	1.00	35.76
ATOM	5171	C	ALA	668	47.548	13.161	25.893	1.00	38.76
ATOM	5172	O	ALA	668	48.000	14.201	25.414	1.00	38.04
ATOM	5173	N	PRO	669	46.416	13.142	26.608	1.00	41.60
ATOM	5174	CD	PRO	669	45.819	11.981	27.282	1.00	41.64
ATOM	5175	CA	PRO	669	45.614	14.347	26.841	1.00	43.25
ATOM	5176	CB	PRO	669	44.478	13.827	27.718	1.00	45.08
ATOM	5177	CG	PRO	669	44.383	12.368	27.325	1.00	44.04
ATOM	5178	C	PRO	669	46.390	15.486	27.526	1.00	44.68
ATOM	5179	O	PRO	669	46.304	16.644	27.111	1.00	43.79
ATOM	5180	N	GLU	670	47.135	15.164	28.580	1.00	44.29
ATOM	5182	CA	GLU	670	47.905	16.195	29.266	1.00	45.36
ATOM	5183	CB	GLU	670	48.596	15.637	30.509	1.00	46.97
ATOM	5184	CG	GLU	670	49.858	14.819	30.243	1.00	50.04
ATOM	5185	CD	GLU	670	49.588	13.345	30.070	1.00	51.35
ATOM	5186	OE1	GLU	670	50.512	12.552	30.327	1.00	50.99
ATOM	5187	OE2	GLU	670	48.458	12.975	29.700	1.00	52.70
ATOM	5188	C	GLU	670	48.942	16.802	28.320	1.00	45.63
ATOM	5189	O	GLU	670	49.174	18.006	28.340	1.00	44.75
ATOM	5190	N	ALA	671	49.546	15.962	27.482	1.00	46.18
ATOM	5192	CA	ALA	671	50.555	16.406	26.531	1.00	46.44
ATOM	5193	CB	ALA	671	51.218	15.203	25.860	1.00	43.27
ATOM	5194	C	ALA	671	49.931	17.313	25.483	1.00	47.85
ATOM	5195	O	ALA	671	50.485	18.355	25.150	1.00	47.61
ATOM	5196	N	LEU	672	48.748	16.928	25.018	1.00	51.40
ATOM	5198	CA	LEU	672	48.010	17.657	23.990	1.00	54.25
ATOM	5199	CB	LEU	672	46.996	16.705	23.346	1.00	55.60
ATOM	5200	CG	LEU	672	46.202	17.113	22.105	1.00	58.92
ATOM	5201	CD1	LEU	672	47.114	17.425	20.932	1.00	58.60
ATOM	5202	CD2	LEU	672	45.269	15.977	21.753	1.00	60.32
ATOM	5203	C	LEU	672	47.315	18.925	24.514	1.00	55.91
ATOM	5204	O	LEU	672	47.289	19.958	23.837	1.00	55.72
ATOM	5205	N	PHE	673	46.782	18.846	25.730	1.00	57.88
ATOM	5207	CA	PHE	673	46.089	19.977	26.342	1.00	60.07
ATOM	5208	CB	PHE	673	44.873	19.484	27.127	1.00	57.08
ATOM	5209	CG	PHE	673	43.876	18.742	26.290	1.00	56.39
ATOM	5210	CD1	PHE	673	43.191	17.653	26.813	1.00	57.67
ATOM	5211	CD2	PHE	673	43.633	19.116	24.970	1.00	55.36
ATOM	5212	CE1	PHE	673	42.281	16.939	26.036	1.00	57.42
ATOM	5213	CE2	PHE	673	42.724	18.410	24.183	1.00	55.91
ATOM	5214	CZ	PHE	673	42.049	17.317	24.720	1.00	56.42
ATOM	5215	C	PHE	673	46.974	20.854	27.238	1.00	63.00

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ATOM	5216	O	PHE	673	46.926	22.085	27.155	1.00	65.31
ATOM	5217	N	ASP	674	47.786	20.223	28.081	1.00	64.08
ATOM	5219	CA	ASP	674	48.656	20.954	28.999	1.00	64.97
ATOM	5220	CB	ASP	674	48.545	20.375	30.409	1.00	65.13
ATOM	5221	CG	ASP	674	47.128	20.358	30.923	1.00	67.33
ATOM	5222	OD1	ASP	674	46.684	19.283	31.372	1.00	66.68
ATOM	5223	OD2	ASP	674	46.462	21.416	30.869	1.00	69.20
ATOM	5224	C	ASP	674	50.132	20.971	28.603	1.00	66.38
ATOM	5225	O	ASP	674	50.984	21.304	29.434	1.00	68.44
ATOM	5226	N	ARG	675	50.441	20.585	27.365	1.00	65.68
ATOM	5228	CA	ARG	675	51.829	20.550	26.883	1.00	63.71
ATOM	5229	CB	ARG	675	52.321	21.970	26.576	1.00	63.67
ATOM	5230	CG	ARG	675	51.491	22.685	25.531	1.00	67.65
ATOM	5231	CD	ARG	675	52.094	24.034	25.146	1.00	73.20
ATOM	5232	NE	ARG	675	53.382	23.911	24.457	1.00	74.09
ATOM	5234	CZ	ARG	675	54.159	24.939	24.122	1.00	73.41
ATOM	5235	NH1	ARG	675	53.788	26.182	24.408	1.00	72.90
ATOM	5238	NH2	ARG	675	55.324	24.720	23.524	1.00	71.96
ATOM	5241	C	ARG	675	52.780	19.864	27.876	1.00	61.41
ATOM	5242	O	ARG	675	53.960	20.208	27.966	1.00	62.62
ATOM	5243	N	ILE	676	52.248	18.903	28.627	1.00	59.15
ATOM	5245	CA	ILE	676	53.016	18.162	29.623	1.00	56.88
ATOM	5246	CB	ILE	676	52.175	17.904	30.891	1.00	56.26
ATOM	5247	CG2	ILE	676	52.871	16.904	31.807	1.00	53.11
ATOM	5248	CG1	ILE	676	51.920	19.224	31.614	1.00	57.86
ATOM	5249	CD1	ILE	676	51.038	19.096	32.835	1.00	61.05
ATOM	5250	C	ILE	676	53.494	16.828	29.070	1.00	56.58
ATOM	5251	O	ILE	676	52.727	15.869	28.985	1.00	58.12
ATOM	5252	N	TYR	677	54.760	16.773	28.680	1.00	54.34
ATOM	5254	CA	TYR	677	55.340	15.556	28.143	1.00	51.14
ATOM	5255	CB	TYR	677	56.240	15.868	26.954	1.00	52.37
ATOM	5256	CG	TYR	677	55.488	16.315	25.719	1.00	56.21
ATOM	5257	CD1	TYR	677	55.187	17.660	25.512	1.00	56.78
ATOM	5258	CE1	TYR	677	54.534	18.086	24.353	1.00	57.54
ATOM	5259	CD2	TYR	677	55.113	15.395	24.738	1.00	57.82
ATOM	5260	CE2	TYR	677	54.458	15.809	23.571	1.00	59.32
ATOM	5261	CZ	TYR	677	54.177	17.159	23.385	1.00	59.59
ATOM	5262	OH	TYR	677	53.557	17.589	22.230	1.00	60.15
ATOM	5264	C	TYR	677	56.124	14.854	29.224	1.00	48.64
ATOM	5265	O	TYR	677	57.040	15.430	29.812	1.00	50.45
ATOM	5266	N	THR	678	55.733	13.621	29.510	1.00	44.59
ATOM	5268	CA	THR	678	56.397	12.834	30.524	1.00	42.21
ATOM	5269	CB	THR	678	55.524	12.726	31.791	1.00	43.55
ATOM	5270	OG1	THR	678	54.302	12.045	31.475	1.00	47.42
ATOM	5272	CG2	THR	678	55.190	14.105	32.327	1.00	48.74
ATOM	5273	C	THR	678	56.634	11.432	29.992	1.00	39.94
ATOM	5274	O	THR	678	56.207	11.085	28.892	1.00	39.34
ATOM	5275	N	HIS	679	57.312	10.616	30.784	1.00	38.54
ATOM	5277	CA	HIS	679	57.532	9.248	30.390	1.00	38.29
ATOM	5278	CB	HIS	679	58.441	8.546	31.391	1.00	39.51
ATOM	5279	CG	HIS	679	59.869	8.997	31.331	1.00	43.13
ATOM	5280	CD2	HIS	679	60.630	9.668	32.233	1.00	43.49
ATOM	5281	ND1	HIS	679	60.694	8.726	30.263	1.00	43.00
ATOM	5283	CE1	HIS	679	61.903	9.201	30.510	1.00	43.62

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ATOM	5284	NE2	HIS	679	61.889	9.778	31.695	1.00	44.68
ATOM	5286	C	HIS	679	56.147	8.599	30.359	1.00	39.42
ATOM	5287	O	HIS	679	55.898	7.667	29.593	1.00	40.00
ATOM	5288	N	GLN	680	55.228	9.156	31.142	1.00	38.96
ATOM	5290	CA	GLN	680	53.867	8.649	31.209	1.00	38.84
ATOM	5291	CB	GLN	680	53.214	9.010	32.543	1.00	40.90
ATOM	5292	CG	GLN	680	53.835	8.278	33.732	1.00	44.42
ATOM	5293	CD	GLN	680	53.677	6.756	33.660	1.00	44.47
ATOM	5294	OE1	GLN	680	52.595	6.225	33.908	1.00	45.52
ATOM	5295	NE2	GLN	680	54.767	6.050	33.348	1.00	42.06
ATOM	5298	C	GLN	680	53.013	9.099	30.036	1.00	38.25
ATOM	5299	O	GLN	680	51.968	8.505	29.758	1.00	39.27
ATOM	5300	N	SER	681	53.427	10.155	29.349	1.00	37.00
ATOM	5302	CA	SER	681	52.665	10.571	28.182	1.00	38.02
ATOM	5303	CB	SER	681	52.929	12.034	27.813	1.00	40.29
ATOM	5304	OG	SER	681	54.307	12.286	27.620	1.00	47.29
ATOM	5306	C	SER	681	53.066	9.620	27.051	1.00	37.43
ATOM	5307	O	SER	681	52.289	9.366	26.136	1.00	37.86
ATOM	5308	N	ASP	682	54.281	9.077	27.162	1.00	35.23
ATOM	5310	CA	ASP	682	54.800	8.106	26.205	1.00	33.24
ATOM	5311	CB	ASP	682	56.284	7.820	26.464	1.00	31.85
ATOM	5312	CG	ASP	682	57.224	8.732	25.677	1.00	34.18
ATOM	5313	OD1	ASP	682	58.445	8.537	25.826	1.00	31.79
ATOM	5314	OD2	ASP	682	56.763	9.620	24.908	1.00	29.15
ATOM	5315	C	ASP	682	54.015	6.810	26.374	1.00	31.52
ATOM	5316	O	ASP	682	53.788	6.087	25.411	1.00	31.93
ATOM	5317	N	VAL	683	53.653	6.499	27.617	1.00	33.14
ATOM	5319	CA	VAL	683	52.879	5.293	27.935	1.00	32.79
ATOM	5320	CB	VAL	683	52.725	5.095	29.478	1.00	34.56
ATOM	5321	CG1	VAL	683	51.653	4.059	29.790	1.00	32.39
ATOM	5322	CG2	VAL	683	54.050	4.649	30.088	1.00	28.08
ATOM	5323	C	VAL	683	51.506	5.338	27.245	1.00	31.45
ATOM	5324	O	VAL	683	51.008	4.311	26.779	1.00	30.37
ATOM	5325	N	TRP	684	50.919	6.531	27.147	1.00	31.04
ATOM	5327	CA	TRP	684	49.638	6.686	26.464	1.00	31.23
ATOM	5328	CB	TRP	684	49.158	8.137	26.525	1.00	34.14
ATOM	5329	CG	TRP	684	47.913	8.423	25.694	1.00	37.17
ATOM	5330	CD2	TRP	684	46.573	8.593	26.187	1.00	38.61
ATOM	5331	CE2	TRP	684	45.755	8.888	25.064	1.00	37.91
ATOM	5332	CE3	TRP	684	45.978	8.528	27.452	1.00	37.63
ATOM	5333	CD1	TRP	684	47.850	8.612	24.337	1.00	37.39
ATOM	5334	NE1	TRP	684	46.560	8.894	23.956	1.00	34.76
ATOM	5336	CZ2	TRP	684	44.380	9.118	25.181	1.00	34.79
ATOM	5337	CZ3	TRP	684	44.611	8.759	27.563	1.00	38.53
ATOM	5338	CH2	TRP	684	43.830	9.048	26.428	1.00	37.59
ATOM	5339	C	TRP	684	49.876	6.294	25.013	1.00	29.99
ATOM	5340	O	TRP	684	49.254	5.356	24.503	1.00	30.82
ATOM	5341	N	SER	685	50.815	6.992	24.380	1.00	28.28
ATOM	5343	CA	SER	685	51.174	6.738	22.986	1.00	27.54
ATOM	5344	CB	SER	685	52.444	7.504	22.631	1.00	26.69
ATOM	5345	OG	SER	685	52.355	8.874	22.986	1.00	32.15
ATOM	5347	C	SER	685	51.399	5.249	22.737	1.00	26.41
ATOM	5348	O	SER	685	50.968	4.709	21.713	1.00	29.52
ATOM	5349	N	PHE	686	52.065	4.582	23.676	1.00	26.47

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ATOM	5351	CA	PHE	686	52.325	3.151	23.563	1.00	26.35
ATOM	5352	CB	PHE	686	53.167	2.668	24.754	1.00	25.01
ATOM	5353	CG	PHE	686	53.447	1.182	24.742	1.00	27.24
ATOM	5354	CD1	PHE	686	54.187	0.600	23.712	1.00	24.88
ATOM	5355	CD2	PHE	686	52.915	0.351	25.729	1.00	24.99
ATOM	5356	CE1	PHE	686	54.389	-0.783	23.655	1.00	22.77
ATOM	5357	CE2	PHE	686	53.113	-1.036	25.679	1.00	28.39
ATOM	5358	CZ	PHE	686	53.853	-1.601	24.631	1.00	22.71
ATOM	5359	C	PHE	686	50.997	2.366	23.466	1.00	28.82
ATOM	5360	O	PHE	686	50.892	1.398	22.696	1.00	26.41
ATOM	5361	N	GLY	687	49.988	2.797	24.229	1.00	29.65
ATOM	5363	CA	GLY	687	48.692	2.134	24.194	1.00	29.88
ATOM	5364	C	GLY	687	48.099	2.158	22.794	1.00	29.57
ATOM	5365	O	GLY	687	47.560	1.165	22.300	1.00	30.38
ATOM	5366	N	VAL	688	48.222	3.310	22.147	1.00	29.19
ATOM	5368	CA	VAL	688	47.718	3.478	20.795	1.00	25.09
ATOM	5369	CB	VAL	688	47.747	4.956	20.359	1.00	22.52
ATOM	5370	CG1	VAL	688	47.106	5.115	18.985	1.00	21.13
ATOM	5371	CG2	VAL	688	47.001	5.810	21.366	1.00	22.50
ATOM	5372	C	VAL	688	48.574	2.636	19.865	1.00	23.82
ATOM	5373	O	VAL	688	48.080	2.132	18.871	1.00	25.39
ATOM	5374	N	LEU	689	49.849	2.463	20.208	1.00	24.46
ATOM	5376	CA	LEU	689	50.764	1.655	19.401	1.00	25.68
ATOM	5377	CB	LEU	689	52.222	1.893	19.834	1.00	25.93
ATOM	5378	CG	LEU	689	53.374	1.307	19.004	1.00	25.01
ATOM	5379	CD1	LEU	689	54.655	2.080	19.257	1.00	25.86
ATOM	5380	CD2	LEU	689	53.593	-0.145	19.318	1.00	24.90
ATOM	5381	C	LEU	689	50.374	0.171	19.531	1.00	26.50
ATOM	5382	O	LEU	689	50.464	-0.578	18.558	1.00	27.13
ATOM	5383	N	LEU	690	49.927	-0.234	20.724	1.00	27.76
ATOM	5385	CA	LEU	690	49.481	-1.610	20.980	1.00	28.59
ATOM	5386	CB	LEU	690	49.087	-1.800	22.447	1.00	30.38
ATOM	5387	CG	LEU	690	50.121	-2.065	23.545	1.00	29.57
ATOM	5388	CD1	LEU	690	49.435	-1.966	24.907	1.00	27.40
ATOM	5389	CD2	LEU	690	50.744	-3.431	23.360	1.00	28.79
ATOM	5390	C	LEU	690	48.242	-1.849	20.134	1.00	28.77
ATOM	5391	O	LEU	690	48.055	-2.922	19.573	1.00	28.07
ATOM	5392	N	TRP	691	47.383	-0.838	20.075	1.00	29.58
ATOM	5394	CA	TRP	691	46.166	-0.921	19.275	1.00	30.53
ATOM	5395	CB	TRP	691	45.327	0.349	19.451	1.00	28.28
ATOM	5396	CG	TRP	691	43.985	0.300	18.769	1.00	25.86
ATOM	5397	CD2	TRP	691	43.702	0.689	17.421	1.00	23.99
ATOM	5398	CE2	TRP	691	42.321	0.498	17.215	1.00	25.08
ATOM	5399	CE3	TRP	691	44.487	1.165	16.367	1.00	20.88
ATOM	5400	CD1	TRP	691	42.791	-0.090	19.314	1.00	23.72
ATOM	5401	NE1	TRP	691	41.786	0.031	18.389	1.00	26.15
ATOM	5403	CZ2	TRP	691	41.704	0.788	15.997	1.00	25.07
ATOM	5404	CZ3	TRP	691	43.883	1.448	15.163	1.00	22.80
ATOM	5405	CH2	TRP	691	42.501	1.251	14.982	1.00	24.95
ATOM	5406	C	TRP	691	46.566	-1.116	17.811	1.00	30.63
ATOM	5407	O	TRP	691	45.943	-1.892	17.093	1.00	33.02
ATOM	5408	N	GLU	692	47.625	-0.431	17.386	1.00	31.00
ATOM	5410	CA	GLU	692	48.130	-0.545	16.018	1.00	29.00
ATOM	5411	CB	GLU	692	49.285	0.426	15.778	1.00	26.55

ATOM	5412	CG	GLU	692	48.873	1.876	15.651	1.00	29.90
ATOM	5413	CD	GLU	692	50.040	2.781	15.316	1.00	29.83
ATOM	5414	OE1	GLU	692	50.770	3.174	16.247	1.00	32.18
ATOM	5415	OE2	GLU	692	50.227	3.110	14.124	1.00	31.57
ATOM	5416	C	GLU	692	48.622	-1.959	15.735	1.00	29.02
ATOM	5417	O	GLU	692	48.474	-2.467	14.627	1.00	29.22
ATOM	5418	N	ILE	693	49.258	-2.573	16.724	1.00	29.54
ATOM	5420	CA	ILE	693	49.766	-3.933	16.555	1.00	31.01
ATOM	5421	CB	ILE	693	50.634	-4.360	17.757	1.00	32.36
ATOM	5422	CG2	ILE	693	51.006	-5.845	17.641	1.00	34.39
ATOM	5423	CG1	ILE	693	51.909	-3.506	17.815	1.00	30.30
ATOM	5424	CD1	ILE	693	52.696	-3.693	19.082	1.00	25.66
ATOM	5425	C	ILE	693	48.638	-4.939	16.381	1.00	30.63
ATOM	5426	O	ILE	693	48.633	-5.738	15.451	1.00	31.10
ATOM	5427	N	PHE	694	47.644	-4.858	17.248	1.00	32.60
ATOM	5429	CA	PHE	694	46.543	-5.793	17.172	1.00	33.86
ATOM	5430	CB	PHE	694	45.938	-5.970	18.563	1.00	35.66
ATOM	5431	CG	PHE	694	46.941	-6.499	19.559	1.00	35.70
ATOM	5432	CD1	PHE	694	47.460	-5.684	20.556	1.00	37.18
ATOM	5433	CD2	PHE	694	47.449	-7.794	19.426	1.00	34.37
ATOM	5434	CE1	PHE	694	48.473	-6.150	21.392	1.00	36.90
ATOM	5435	CE2	PHE	694	48.456	-8.265	20.255	1.00	31.89
ATOM	5436	CZ	PHE	694	48.970	-7.446	21.234	1.00	34.95
ATOM	5437	C	PHE	694	45.532	-5.576	16.049	1.00	34.26
ATOM	5438	O	PHE	694	44.702	-6.442	15.787	1.00	37.52
ATOM	5439	N	THR	695	45.636	-4.441	15.359	1.00	32.23
ATOM	5441	CA	THR	695	44.775	-4.160	14.215	1.00	28.08
ATOM	5442	CB	THR	695	44.186	-2.728	14.241	1.00	25.71
ATOM	5443	OG1	THR	695	45.237	-1.762	14.228	1.00	24.94
ATOM	5445	CG2	THR	695	43.353	-2.528	15.468	1.00	23.07
ATOM	5446	C	THR	695	45.615	-4.348	12.955	1.00	27.53
ATOM	5447	O	THR	695	45.166	-4.066	11.845	1.00	30.89
ATOM	5448	N	LEU	696	46.833	-4.848	13.145	1.00	27.73
ATOM	5450	CA	LEU	696	47.781	-5.081	12.061	1.00	28.99
ATOM	5451	CB	LEU	696	47.370	-6.297	11.226	1.00	27.78
ATOM	5452	CG	LEU	696	47.379	-7.591	12.047	1.00	29.89
ATOM	5453	CD1	LEU	696	47.251	-8.823	11.164	1.00	29.96
ATOM	5454	CD2	LEU	696	48.668	-7.656	12.803	1.00	30.20
ATOM	5455	C	LEU	696	48.044	-3.853	11.179	1.00	30.33
ATOM	5456	O	LEU	696	48.006	-3.926	9.948	1.00	29.41
ATOM	5457	N	GLY	697	48.374	-2.738	11.831	1.00	30.92
ATOM	5459	CA	GLY	697	48.655	-1.503	11.113	1.00	30.35
ATOM	5460	C	GLY	697	47.420	-0.650	10.912	1.00	30.65
ATOM	5461	O	GLY	697	47.359	0.178	10.000	1.00	30.01
ATOM	5462	N	GLY	698	46.428	-0.836	11.772	1.00	30.50
ATOM	5464	CA	GLY	698	45.209	-0.063	11.656	1.00	30.36
ATOM	5465	C	GLY	698	45.416	1.415	11.930	1.00	30.07
ATOM	5466	O	GLY	698	46.320	1.809	12.666	1.00	30.56
ATOM	5467	N	SER	699	44.554	2.228	11.338	1.00	29.65
ATOM	5469	CA	SER	699	44.597	3.674	11.485	1.00	28.42
ATOM	5470	CB	SER	699	44.263	4.324	10.145	1.00	24.61
ATOM	5471	OG	SER	699	43.960	5.693	10.280	1.00	31.25
ATOM	5473	C	SER	699	43.621	4.137	12.574	1.00	28.27
ATOM	5474	O	SER	699	42.406	3.930	12.474	1.00	27.14

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ATOM	5475	N	PRO	700	44.160	4.682	13.675	1.00	29.29
ATOM	5476	CD	PRO	700	45.587	4.867	13.999	1.00	26.09
ATOM	5477	CA	PRO	700	43.303	5.155	14.764	1.00	29.30
ATOM	5478	CB	PRO	700	44.319	5.624	15.812	1.00	27.68
ATOM	5479	CG	PRO	700	45.531	5.982	14.985	1.00	27.85
ATOM	5480	C	PRO	700	42.413	6.305	14.306	1.00	29.71
ATOM	5481	O	PRO	700	42.800	7.096	13.446	1.00	31.38
ATOM	5482	N	TYR	701	41.204	6.357	14.854	1.00	29.51
ATOM	5484	CA	TYR	701	40.246	7.419	14.548	1.00	30.25
ATOM	5485	CB	TYR	701	40.559	8.647	15.405	1.00	33.50
ATOM	5486	CG	TYR	701	40.321	8.413	16.866	1.00	37.84
ATOM	5487	CD1	TYR	701	41.323	8.638	17.803	1.00	40.05
ATOM	5488	CE1	TYR	701	41.092	8.412	19.158	1.00	42.28
ATOM	5489	CD2	TYR	701	39.084	7.965	17.310	1.00	41.54
ATOM	5490	CE2	TYR	701	38.845	7.738	18.653	1.00	43.70
ATOM	5491	CZ	TYR	701	39.845	7.963	19.574	1.00	42.63
ATOM	5492	OH	TYR	701	39.584	7.716	20.907	1.00	45.31
ATOM	5494	C	TYR	701	40.173	7.829	13.088	1.00	28.45
ATOM	5495	O	TYR	701	40.356	9.001	12.760	1.00	29.03
ATOM	5496	N	PRO	702	39.901	6.867	12.191	1.00	28.05
ATOM	5497	CD	PRO	702	39.671	5.430	12.417	1.00	26.90
ATOM	5498	CA	PRO	702	39.815	7.181	10.764	1.00	27.48
ATOM	5499	CB	PRO	702	39.610	5.807	10.119	1.00	27.06
ATOM	5500	CG	PRO	702	38.923	5.036	11.169	1.00	28.28
ATOM	5501	C	PRO	702	38.689	8.145	10.440	1.00	26.81
ATOM	5502	O	PRO	702	37.554	7.953	10.865	1.00	26.26
ATOM	5503	N	GLY	703	39.035	9.192	9.693	1.00	28.48
ATOM	5505	CA	GLY	703	38.085	10.217	9.295	1.00	26.54
ATOM	5506	C	GLY	703	37.862	11.285	10.351	1.00	28.03
ATOM	5507	O	GLY	703	37.110	12.231	10.108	1.00	28.93
ATOM	5508	N	VAL	704	38.518	11.149	11.505	1.00	28.16
ATOM	5510	CA	VAL	704	38.369	12.081	12.619	1.00	29.55
ATOM	5511	CB	VAL	704	38.473	11.360	13.984	1.00	28.50
ATOM	5512	CG1	VAL	704	38.330	12.350	15.135	1.00	28.07
ATOM	5513	CG2	VAL	704	37.403	10.295	14.091	1.00	29.78
ATOM	5514	C	VAL	704	39.375	13.227	12.588	1.00	32.00
ATOM	5515	O	VAL	704	40.578	13.028	12.758	1.00	33.85
ATOM	5516	N	PRO	705	38.888	14.446	12.336	1.00	33.56
ATOM	5517	CD	PRO	705	37.512	14.763	11.906	1.00	33.69
ATOM	5518	CA	PRO	705	39.745	15.628	12.280	1.00	32.65
ATOM	5519	CB	PRO	705	38.863	16.647	11.569	1.00	34.10
ATOM	5520	CG	PRO	705	37.478	16.256	12.021	1.00	36.38
ATOM	5521	C	PRO	705	40.164	16.081	13.668	1.00	33.22
ATOM	5522	O	PRO	705	39.549	15.708	14.668	1.00	33.26
ATOM	5523	N	VAL	706	41.198	16.912	13.710	1.00	34.61
ATOM	5525	CA	VAL	706	41.764	17.417	14.954	1.00	37.72
ATOM	5526	CB	VAL	706	42.803	18.527	14.673	1.00	39.14
ATOM	5527	CG1	VAL	706	43.483	18.941	15.957	1.00	39.12
ATOM	5528	CG2	VAL	706	43.836	18.038	13.670	1.00	41.07
ATOM	5529	C	VAL	706	40.740	17.934	15.969	1.00	38.70
ATOM	5530	O	VAL	706	40.761	17.536	17.136	1.00	38.42
ATOM	5531	N	GLU	707	39.834	18.796	15.517	1.00	40.43
ATOM	5533	CA	GLU	707	38.823	19.375	16.395	1.00	40.66
ATOM	5534	CB	GLU	707	37.973	20.379	15.621	1.00	43.40

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ATOM	5535	C	GLU	707	37.940	18.316	17.028	1.00	41.03
ATOM	5536	O	GLU	707	37.642	18.370	18.231	1.00	41.52
ATOM	5537	N	GLU	708	37.560	17.327	16.224	1.00	41.62
ATOM	5539	CA	GLU	708	36.708	16.243	16.700	1.00	41.06
ATOM	5541	CB	GLU	708	36.179	15.425	15.523	1.00	45.19
ATOM	5542	CG	GLU	708	35.281	16.221	14.571	1.00	48.74
ATOM	5543	OE1	GLU	708	34.063	16.825	15.258	1.00	57.18
ATOM	5544	OE2	GLU	708	33.523	16.203	16.207	1.00	54.30
ATOM	5545	C	GLU	708	33.646	17.934	14.837	1.00	61.76
ATOM	5546	O	GLU	708	37.443	15.363	17.694	1.00	38.39
ATOM	5547	N	LEU	709	36.867	14.927	18.696	1.00	36.76
ATOM	5549	CA	LEU	709	38.725	15.131	17.434	1.00	37.78
ATOM	5550	CB	LEU	709	39.555	14.327	18.324	1.00	38.13
ATOM	5551	CG	LEU	709	41.007	14.255	17.820	1.00	35.45
ATOM	5552	CD1	LEU	709	41.984	13.560	18.786	1.00	35.57
ATOM	5553	CD2	LEU	709	41.825	12.049	18.729	1.00	32.33
ATOM	5554	C	LEU	709	43.407	13.965	18.484	1.00	31.98
ATOM	5555	O	LEU	709	39.550	14.946	19.716	1.00	38.31
ATOM	5556	N	PHE	710	39.362	14.250	20.717	1.00	38.16
ATOM	5558	CA	PHE	710	39.776	16.254	19.770	1.00	40.09
ATOM	5559	CB	PHE	710	39.807	16.973	21.036	1.00	43.61
ATOM	5560	CG	PHE	710	39.997	18.475	20.797	1.00	48.22
ATOM	5561	CD1	PHE	710	41.328	18.834	20.192	1.00	51.77
ATOM	5562	CD2	PHE	710	42.395	17.939	20.231	1.00	52.94
ATOM	5563	CE1	PHE	710	41.513	20.072	19.579	1.00	53.99
ATOM	5564	CE2	PHE	710	43.632	18.275	19.679	1.00	56.48
ATOM	5565	CZ	PHE	710	42.746	20.422	19.021	1.00	55.72
ATOM	5566	C	PHE	710	43.807	19.517	19.069	1.00	57.84
ATOM	5567	O	PHE	710	38.519	16.726	21.796	1.00	43.35
ATOM	5568	N	LYS	711	38.539	16.424	22.989	1.00	43.22
ATOM	5570	CA	LYS	711	37.399	16.804	21.083	1.00	44.68
ATOM	5571	CB	LYS	711	36.095	16.587	21.690	1.00	43.47
ATOM	5572	CG	LYS	711	34.977	16.878	20.687	1.00	44.33
ATOM	5573	CD	LYS	711	33.601	16.765	21.299	1.00	47.63
ATOM	5574	CE	LYS	711	32.510	17.206	20.362	1.00	49.97
ATOM	5575	NZ	LYS	711	31.158	16.873	20.960	1.00	51.70
ATOM	5579	C	LYS	711	30.038	17.412	20.150	1.00	57.55
ATOM	5580	O	LYS	711	35.986	15.173	22.261	1.00	42.72
ATOM	5581	N	LEU	712	35.589	14.999	23.420	1.00	41.16
ATOM	5583	CA	LEU	712	36.392	14.176	21.471	1.00	42.52
ATOM	5584	CB	LEU	712	36.361	12.770	21.898	1.00	42.52
ATOM	5585	CG	LEU	712	36.922	11.843	20.809	1.00	41.56
ATOM	5586	CD1	LEU	712	36.090	11.528	19.560	1.00	41.87
ATOM	5587	CD2	LEU	712	36.902	10.620	18.636	1.00	36.28
ATOM	5588	C	LEU	712	34.760	10.868	19.951	1.00	37.19
ATOM	5589	O	LEU	712	37.158	12.564	23.180	1.00	42.34
ATOM	5590	N	LEU	713	36.697	11.886	24.107	1.00	40.77
ATOM	5592	CA	LEU	713	38.366	13.121	23.208	1.00	42.68
ATOM	5593	CB	LEU	713	39.240	13.025	24.371	1.00	44.05
ATOM	5594	CG	LEU	713	40.581	13.710	24.100	1.00	45.45
ATOM	5595	CD1	LEU	713	41.418	13.114	22.963	1.00	44.78
ATOM	5596	CD2	LEU	713	42.676	13.945	22.750	1.00	41.89
ATOM	5597	C	LEU	713	41.757	11.660	23.282	1.00	43.21
					38.571	13.654	25.591	1.00	44.66

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ATOM	5598	O	LEU	713	38.562	13.051	26.662	1.00	45.70
ATOM	5599	N	LYS	714	37.980	14.839	25.418	1.00	43.05
ATOM	5601	CA	LYS	714	37.300	15.510	26.524	1.00	42.19
ATOM	5602	CB	LYS	714	36.884	16.921	26.127	1.00	42.41
ATOM	5603	CG	LYS	714	38.076	17.828	25.918	1.00	46.10
ATOM	5604	CD	LYS	714	37.684	19.259	25.589	1.00	49.86
ATOM	5605	CE	LYS	714	38.939	20.097	25.292	1.00	52.55
ATOM	5606	NZ	LYS	714	39.889	20.148	26.459	1.00	50.17
ATOM	5610	C	LYS	714	36.104	14.728	27.054	1.00	42.39
ATOM	5611	O	LYS	714	35.767	14.824	28.237	1.00	43.44
ATOM	5612	N	GLU	715	35.480	13.934	26.192	1.00	40.44
ATOM	5614	CA	GLU	715	34.342	13.118	26.593	1.00	37.90
ATOM	5615	CB	GLU	715	33.408	12.893	25.411	1.00	39.54
ATOM	5616	CG	GLU	715	32.800	14.174	24.846	1.00	45.20
ATOM	5617	CD	GLU	715	32.032	13.936	23.563	1.00	47.85
ATOM	5618	OE1	GLU	715	32.409	13.008	22.810	1.00	50.00
ATOM	5619	OE2	GLU	715	31.061	14.677	23.304	1.00	50.41
ATOM	5620	C	GLU	715	34.793	11.773	27.157	1.00	37.31
ATOM	5621	O	GLU	715	33.970	10.907	27.450	1.00	36.79
ATOM	5622	N	GLY	716	36.102	11.585	27.286	1.00	36.60
ATOM	5624	CA	GLY	716	36.623	10.336	27.819	1.00	37.11
ATOM	5625	C	GLY	716	36.503	9.140	26.887	1.00	38.30
ATOM	5626	O	GLY	716	36.603	7.994	27.340	1.00	36.84
ATOM	5627	N	HIS	717	36.307	9.404	25.592	1.00	40.24
ATOM	5629	CA	HIS	717	36.167	8.353	24.579	1.00	42.63
ATOM	5630	CB	HIS	717	35.800	8.951	23.217	1.00	43.11
ATOM	5631	CG	HIS	717	35.745	7.941	22.112	1.00	44.69
ATOM	5632	CD2	HIS	717	34.756	7.101	21.717	1.00	45.13
ATOM	5633	ND1	HIS	717	36.818	7.683	21.283	1.00	47.31
ATOM	5635	CE1	HIS	717	36.494	6.728	20.426	1.00	47.61
ATOM	5636	NE2	HIS	717	35.250	6.357	20.670	1.00	44.95
ATOM	5638	C	HIS	717	37.451	7.567	24.413	1.00	44.84
ATOM	5639	O	HIS	717	38.528	8.152	24.295	1.00	46.79
ATOM	5640	N	ARG	718	37.313	6.247	24.337	1.00	45.44
ATOM	5642	CA	ARG	718	38.440	5.345	24.170	1.00	45.36
ATOM	5643	CB	ARG	718	38.614	4.496	25.434	1.00	43.82
ATOM	5644	CG	ARG	718	38.976	5.308	26.687	1.00	44.52
ATOM	5645	CD	ARG	718	40.284	6.065	26.476	1.00	45.02
ATOM	5646	NE	ARG	718	40.718	6.856	27.630	1.00	43.12
ATOM	5648	CZ	ARG	718	40.550	8.173	27.744	1.00	44.77
ATOM	5649	NH1	ARG	718	39.940	8.859	26.784	1.00	44.67
ATOM	5652	NH2	ARG	718	41.067	8.826	28.777	1.00	46.39
ATOM	5655	C	ARG	718	38.124	4.474	22.952	1.00	45.94
ATOM	5656	O	ARG	718	36.953	4.243	22.645	1.00	47.59
ATOM	5657	N	MET	719	39.145	4.077	22.204	1.00	45.34
ATOM	5659	CA	MET	719	38.925	3.253	21.029	1.00	44.28
ATOM	5660	CB	MET	719	40.198	3.125	20.185	1.00	42.30
ATOM	5661	CG	MET	719	40.575	4.399	19.441	1.00	38.44
ATOM	5662	SD	MET	719	42.000	4.225	18.368	1.00	36.97
ATOM	5663	CE	MET	719	43.317	4.219	19.511	1.00	36.09
ATOM	5664	C	MET	719	38.415	1.877	21.418	1.00	46.21
ATOM	5665	O	MET	719	38.708	1.393	22.517	1.00	43.29
ATOM	5666	N	ASP	720	37.659	1.267	20.498	1.00	48.79
ATOM	5668	CA	ASP	720	37.069	-0.063	20.666	1.00	48.87

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ATOM	5669	CB	ASP	720	36.099	-0.369	19.513	1.00	54.01
ATOM	5670	CG	ASP	720	34.766	0.374	19.632	1.00	59.30
ATOM	5671	OD1	ASP	720	34.762	1.583	19.981	1.00	62.96
ATOM	5672	OD2	ASP	720	33.716	-0.259	19.354	1.00	58.64
ATOM	5673	C	ASP	720	38.126	-1.154	20.688	1.00	46.10
ATOM	5674	O	ASP	720	39.213	-0.992	20.125	1.00	44.13
ATOM	5675	N	LYS	721	37.788	-2.272	21.322	1.00	45.27
ATOM	5677	CA	LYS	721	38.689	-3.413	21.404	1.00	43.25
ATOM	5678	CB	LYS	721	38.172	-4.436	22.416	1.00	42.02
ATOM	5679	CG	LYS	721	39.072	-5.651	22.557	1.00	46.57
ATOM	5680	CD	LYS	721	38.602	-6.576	23.666	1.00	49.96
ATOM	5681	CE	LYS	721	38.300	-7.971	23.141	1.00	51.80
ATOM	5682	NZ	LYS	721	37.937	-8.920	24.240	1.00	56.08
ATOM	5686	C	LYS	721	38.769	-4.055	20.031	1.00	43.67
ATOM	5687	O	LYS	721	37.736	-4.313	19.394	1.00	44.02
ATOM	5688	N	PRO	722	39.995	-4.233	19.513	1.00	43.94
ATOM	5689	CD	PRO	722	41.281	-3.711	20.001	1.00	45.90
ATOM	5690	CA	PRO	722	40.159	-4.853	18.198	1.00	43.96
ATOM	5691	CB	PRO	722	41.665	-4.720	17.941	1.00	43.11
ATOM	5692	CG	PRO	722	42.046	-3.509	18.715	1.00	45.16
ATOM	5693	C	PRO	722	39.772	-6.317	18.295	1.00	43.09
ATOM	5694	O	PRO	722	39.764	-6.888	19.385	1.00	41.32
ATOM	5695	N	SER	723	39.382	-6.902	17.170	1.00	45.79
ATOM	5697	CA	SER	723	39.044	-8.316	17.144	1.00	46.67
ATOM	5698	CB	SER	723	38.303	-8.664	15.857	1.00	44.69
ATOM	5699	OG	SER	723	39.131	-8.414	14.736	1.00	49.79
ATOM	5701	C	SER	723	40.422	-8.961	17.148	1.00	46.90
ATOM	5702	O	SER	723	41.360	-8.411	16.581	1.00	48.81
ATOM	5703	N	ASN	724	40.540	-10.131	17.760	1.00	49.28
ATOM	5705	CA	ASN	724	41.826	-10.804	17.849	1.00	52.10
ATOM	5706	CB	ASN	724	42.480	-10.947	16.469	1.00	55.86
ATOM	5707	CG	ASN	724	41.774	-11.957	15.592	1.00	58.72
ATOM	5708	OD1	ASN	724	41.686	-13.140	15.941	1.00	62.28
ATOM	5709	ND2	ASN	724	41.258	-11.503	14.449	1.00	59.56
ATOM	5712	C	ASN	724	42.665	-9.931	18.770	1.00	51.97
ATOM	5713	O	ASN	724	43.621	-9.274	18.369	1.00	53.85
ATOM	5714	N	CYS	725	42.202	-9.859	20.004	1.00	51.02
ATOM	5716	CA	CYS	725	42.853	-9.094	21.049	1.00	50.18
ATOM	5717	CB	CYS	725	42.708	-7.583	20.811	1.00	47.75
ATOM	5718	SG	CYS	725	43.424	-6.577	22.130	1.00	44.37
ATOM	5719	C	CYS	725	42.131	-9.507	22.315	1.00	49.31
ATOM	5720	O	CYS	725	40.916	-9.371	22.417	1.00	49.90
ATOM	5721	N	THR	726	42.866	-10.088	23.249	1.00	48.52
ATOM	5723	CA	THR	726	42.262	-10.541	24.490	1.00	49.58
ATOM	5724	CB	THR	726	43.251	-11.444	25.291	1.00	49.84
ATOM	5725	OG1	THR	726	44.236	-10.648	25.976	1.00	49.05
ATOM	5727	CG2	THR	726	43.982	-12.363	24.352	1.00	47.96
ATOM	5728	C	THR	726	41.788	-9.369	25.356	1.00	49.93
ATOM	5729	O	THR	726	42.305	-8.256	25.244	1.00	51.55
ATOM	5730	N	ASN	727	40.829	-9.622	26.242	1.00	50.48
ATOM	5732	CA	ASN	727	40.335	-8.577	27.144	1.00	52.17
ATOM	5733	CB	ASN	727	39.190	-9.099	28.016	1.00	57.57
ATOM	5734	CG	ASN	727	39.533	-10.409	28.714	1.00	66.49
ATOM	5735	OD1	ASN	727	40.709	-10.786	28.833	1.00	70.43

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ATOM	5736	ND2	ASN	727	38.500	-11.122	29.175	1.00	68.43
ATOM	5739	C	ASN	727	41.491	-8.091	28.023	1.00	50.29
ATOM	5740	O	ASN	727	41.467	-6.976	28.540	1.00	49.88
ATOM	5741	N	GLU	728	42.518	-8.927	28.163	1.00	50.60
ATOM	5743	CA	GLU	728	43.700	-8.597	28.956	1.00	49.33
ATOM	5744	CB	GLU	728	44.529	-9.859	29.220	1.00	50.44
ATOM	5745	CG	GLU	728	45.802	-9.600	30.008	1.00	55.30
ATOM	5746	CD	GLU	728	46.577	-10.862	30.354	1.00	57.40
ATOM	5747	OE1	GLU	728	46.716	-11.754	29.489	1.00	56.75
ATOM	5748	OE2	GLU	728	47.062	-10.950	31.502	1.00	59.85
ATOM	5749	C	GLU	728	44.539	-7.552	28.212	1.00	47.08
ATOM	5750	O	GLU	728	44.888	-6.512	28.776	1.00	48.02
ATOM	5751	N	LEU	729	44.846	-7.821	26.945	1.00	43.34
ATOM	5753	CA	LEU	729	45.630	-6.891	26.129	1.00	42.01
ATOM	5754	CB	LEU	729	45.899	-7.500	24.751	1.00	39.46
ATOM	5755	CG	LEU	729	46.911	-8.639	24.772	1.00	40.31
ATOM	5756	CD1	LEU	729	46.782	-9.482	23.531	1.00	42.21
ATOM	5757	CD2	LEU	729	48.314	-8.068	24.900	1.00	42.49
ATOM	5758	C	LEU	729	44.901	-5.557	25.980	1.00	40.61
ATOM	5759	O	LEU	729	45.510	-4.481	25.953	1.00	38.33
ATOM	5760	N	TYR	730	43.580	-5.637	25.909	1.00	39.07
ATOM	5762	CA	TYR	730	42.761	-4.455	25.773	1.00	38.61
ATOM	5763	CB	TYR	730	41.341	-4.837	25.369	1.00	36.79
ATOM	5764	CG	TYR	730	40.454	-3.646	25.125	1.00	37.08
ATOM	5765	CD1	TYR	730	40.760	-2.721	24.127	1.00	32.86
ATOM	5766	CE1	TYR	730	39.961	-1.616	23.912	1.00	29.79
ATOM	5767	CD2	TYR	730	39.328	-3.420	25.916	1.00	36.99
ATOM	5768	CE2	TYR	730	38.522	-2.312	25.704	1.00	36.69
ATOM	5769	CZ	TYR	730	38.853	-1.412	24.706	1.00	32.69
ATOM	5770	OH	TYR	730	38.044	-0.320	24.492	1.00	38.80
ATOM	5772	C	TYR	730	42.767	-3.662	27.080	1.00	39.75
ATOM	5773	O	TYR	730	42.781	-2.430	27.065	1.00	40.53
ATOM	5774	N	MET	731	42.738	-4.360	28.210	1.00	41.88
ATOM	5776	CA	MET	731	42.778	-3.684	29.509	1.00	45.34
ATOM	5777	CB	MET	731	42.658	-4.697	30.646	1.00	53.46
ATOM	5778	CG	MET	731	41.253	-5.248	30.836	1.00	64.30
ATOM	5779	SD	MET	731	40.134	-4.095	31.653	1.00	75.78
ATOM	5780	CE	MET	731	40.657	-4.338	33.370	1.00	69.70
ATOM	5781	C	MET	731	44.099	-2.927	29.614	1.00	41.53
ATOM	5782	O	MET	731	44.157	-1.814	30.138	1.00	37.91
ATOM	5783	N	MET	732	45.156	-3.545	29.098	1.00	40.48
ATOM	5785	CA	MET	732	46.478	-2.937	29.091	1.00	40.23
ATOM	5786	CB	MET	732	47.508	-3.872	28.436	1.00	40.29
ATOM	5787	CG	MET	732	48.929	-3.307	28.390	1.00	38.07
ATOM	5788	SD	MET	732	50.171	-4.522	27.908	1.00	37.65
ATOM	5789	CE	MET	732	50.407	-5.343	29.431	1.00	37.90
ATOM	5790	C	MET	732	46.378	-1.623	28.317	1.00	38.96
ATOM	5791	O	MET	732	46.843	-0.591	28.790	1.00	41.36
ATOM	5792	N	MET	733	45.744	-1.663	27.148	1.00	36.94
ATOM	5794	CA	MET	733	45.574	-0.463	26.340	1.00	35.19
ATOM	5795	CB	MET	733	44.796	-0.769	25.070	1.00	36.07
ATOM	5796	CG	MET	733	45.549	-1.577	24.048	1.00	35.99
ATOM	5797	SD	MET	733	44.471	-1.851	22.641	1.00	40.05
ATOM	5798	CE	MET	733	45.244	-3.351	21.909	1.00	33.13

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ATOM	5799	C	MET	733	44.800	0.560	27.141	1.00	37.29
ATOM	5800	O	MET	733	45.207	1.719	27.245	1.00	39.14
ATOM	5801	N	ARG	734	43.690	0.125	27.735	1.00	38.76
ATOM	5803	CA	ARG	734	42.849	1.014	28.532	1.00	39.49
ATOM	5804	CB	ARG	734	41.577	0.297	28.993	1.00	40.33
ATOM	5805	CG	ARG	734	40.699	-0.225	27.856	1.00	38.02
ATOM	5806	CD	ARG	734	40.256	0.877	26.909	1.00	42.72
ATOM	5807	NE	ARG	734	39.443	1.898	27.567	1.00	48.85
ATOM	5809	CZ	ARG	734	38.120	1.838	27.700	1.00	52.35
ATOM	5810	NH1	ARG	734	37.435	0.811	27.222	1.00	54.79
ATOM	5813	NH2	ARG	734	37.477	2.804	28.338	1.00	54.69
ATOM	5816	C	ARG	734	43.627	1.587	29.715	1.00	38.70
ATOM	5817	O	ARG	734	43.445	2.757	30.068	1.00	40.92
ATOM	5818	N	ASP	735	44.530	0.782	30.276	1.00	38.76
ATOM	5820	CA	ASP	735	45.379	1.208	31.399	1.00	38.60
ATOM	5821	CB	ASP	735	46.325	0.087	31.825	1.00	41.34
ATOM	5822	CG	ASP	735	45.622	-1.022	32.574	1.00	44.66
ATOM	5823	OD1	ASP	735	46.048	-2.194	32.428	1.00	43.15
ATOM	5824	OD2	ASP	735	44.657	-0.713	33.313	1.00	44.46
ATOM	5825	C	ASP	735	46.215	2.385	30.938	1.00	37.76
ATOM	5826	O	ASP	735	46.235	3.446	31.585	1.00	36.35
ATOM	5827	N	CYS	736	46.890	2.182	29.805	1.00	35.39
ATOM	5829	CA	CYS	736	47.730	3.196	29.181	1.00	34.77
ATOM	5830	CB	CYS	736	48.379	2.652	27.916	1.00	30.62
ATOM	5831	SG	CYS	736	49.453	1.261	28.198	1.00	30.96
ATOM	5832	C	CYS	736	46.938	4.429	28.814	1.00	35.98
ATOM	5833	O	CYS	736	47.516	5.491	28.606	1.00	37.38
ATOM	5834	N	TRP	737	45.620	4.290	28.713	1.00	38.50
ATOM	5836	CA	TRP	737	44.772	5.423	28.370	1.00	40.16
ATOM	5837	CB	TRP	737	43.791	5.028	27.271	1.00	38.41
ATOM	5838	CG	TRP	737	44.453	4.586	26.011	1.00	39.33
ATOM	5839	CD2	TRP	737	43.893	3.718	25.020	1.00	39.64
ATOM	5840	CE2	TRP	737	44.852	3.583	23.992	1.00	39.97
ATOM	5841	CE3	TRP	737	42.672	3.040	24.900	1.00	37.06
ATOM	5842	CD1	TRP	737	45.695	4.932	25.556	1.00	39.56
ATOM	5843	NE1	TRP	737	45.941	4.336	24.343	1.00	38.61
ATOM	5845	CZ2	TRP	737	44.627	2.795	22.859	1.00	38.78
ATOM	5846	CZ3	TRP	737	42.452	2.261	23.778	1.00	38.90
ATOM	5847	CH2	TRP	737	43.426	2.145	22.772	1.00	38.18
ATOM	5848	C	TRP	737	44.028	6.029	29.563	1.00	41.30
ATOM	5849	O	TRP	737	42.979	6.658	29.398	1.00	41.45
ATOM	5850	N	HIS	738	44.575	5.873	30.763	1.00	43.01
ATOM	5852	CA	HIS	738	43.932	6.423	31.948	1.00	44.64
ATOM	5853	CB	HIS	738	44.454	5.735	33.205	1.00	46.20
ATOM	5854	CG	HIS	738	43.742	6.154	34.458	1.00	50.35
ATOM	5855	CD2	HIS	738	43.473	7.379	34.963	1.00	49.09
ATOM	5856	ND1	HIS	738	43.220	5.244	35.355	1.00	49.94
ATOM	5858	CE1	HIS	738	42.659	5.899	36.357	1.00	52.92
ATOM	5859	NE2	HIS	738	42.798	7.194	36.146	1.00	46.91
ATOM	5861	C	HIS	738	44.174	7.921	32.037	1.00	45.26
ATOM	5862	O	HIS	738	45.314	8.356	32.021	1.00	45.31
ATOM	5863	N	ALA	739	43.099	8.686	32.224	1.00	46.61
ATOM	5865	CA	ALA	739	43.155	10.150	32.322	1.00	48.49
ATOM	5866	CB	ALA	739	41.823	10.681	32.790	1.00	49.69

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ATOM	5867	C	ALA	739	44.272	10.682	33.224	1.00	50.77
ATOM	5868	O	ALA	739	45.004	11.601	32.846	1.00	51.77
ATOM	5869	N	VAL	740	44.336	10.138	34.439	1.00	51.47
ATOM	5871	CA	VAL	740	45.352	10.485	35.439	1.00	51.09
ATOM	5872	CB	VAL	740	44.897	10.075	36.850	1.00	52.40
ATOM	5873	CG1	VAL	740	45.847	10.624	37.878	1.00	53.38
ATOM	5874	CG2	VAL	740	43.485	10.544	37.105	1.00	55.18
ATOM	5875	C	VAL	740	46.649	9.727	35.130	1.00	48.99
ATOM	5876	O	VAL	740	46.773	8.534	35.440	1.00	47.72
ATOM	5877	N	PRO	741	47.646	10.421	34.565	1.00	48.31
ATOM	5878	CD	PRO	741	47.603	11.861	34.253	1.00	47.84
ATOM	5879	CA	PRO	741	48.949	9.852	34.197	1.00	48.51
ATOM	5880	CB	PRO	741	49.762	11.087	33.828	1.00	46.83
ATOM	5881	CG	PRO	741	48.714	12.000	33.255	1.00	46.21
ATOM	5882	C	PRO	741	49.641	9.016	35.275	1.00	49.12
ATOM	5883	O	PRO	741	50.449	8.139	34.955	1.00	46.57
ATOM	5884	N	SER	742	49.327	9.290	36.541	1.00	49.47
ATOM	5886	CA	SER	742	49.928	8.557	37.651	1.00	49.50
ATOM	5887	CB	SER	742	49.760	9.326	38.963	1.00	51.06
ATOM	5888	OG	SER	742	48.403	9.638	39.209	1.00	53.81
ATOM	5890	C	SER	742	49.339	7.159	37.787	1.00	48.81
ATOM	5891	O	SER	742	49.926	6.284	38.427	1.00	49.45
ATOM	5892	N	GLN	743	48.164	6.959	37.203	1.00	47.82
ATOM	5894	CA	GLN	743	47.529	5.658	37.273	1.00	46.34
ATOM	5895	CB	GLN	743	46.022	5.791	37.432	1.00	49.74
ATOM	5896	CG	GLN	743	45.519	5.305	38.784	1.00	55.41
ATOM	5897	CD	GLN	743	46.178	5.030	39.947	1.00	59.15
ATOM	5898	OE1	GLN	743	46.905	5.425	40.748	1.00	59.02
ATOM	5899	NE2	GLN	743	45.922	7.338	40.052	1.00	60.03
ATOM	5902	C	GLN	743	47.874	4.768	36.095	1.00	44.34
ATOM	5903	O	GLN	743	47.548	3.578	36.114	1.00	44.64
ATOM	5904	N	ARG	744	48.497	5.339	35.059	1.00	42.83
ATOM	5906	CA	ARG	744	48.914	4.559	33.880	1.00	40.34
ATOM	5907	CB	ARG	744	49.349	5.469	32.724	1.00	35.84
ATOM	5908	CG	ARG	744	48.296	6.406	32.190	1.00	28.25
ATOM	5909	CD	ARG	744	48.906	7.383	31.216	1.00	22.56
ATOM	5910	NE	ARG	744	47.948	8.437	30.922	1.00	28.09
ATOM	5912	CZ	ARG	744	48.258	9.658	30.493	1.00	32.83
ATOM	5913	NH1	ARG	744	49.524	10.001	30.278	1.00	34.44
ATOM	5916	NH2	ARG	744	47.307	10.569	30.360	1.00	32.00
ATOM	5919	C	ARG	744	50.110	3.712	34.295	1.00	41.58
ATOM	5920	O	ARG	744	50.906	4.124	35.145	1.00	45.48
ATOM	5921	N	PRO	745	50.223	2.489	33.754	1.00	40.97
ATOM	5922	CD	PRO	745	49.345	1.749	32.831	1.00	39.90
ATOM	5923	CA	PRO	745	51.381	1.685	34.157	1.00	39.77
ATOM	5924	CB	PRO	745	51.063	0.311	33.558	1.00	39.31
ATOM	5925	CG	PRO	745	50.255	0.642	32.344	1.00	40.98
ATOM	5926	C	PRO	745	52.664	2.269	33.573	1.00	38.44
ATOM	5927	O	PRO	745	52.631	3.009	32.595	1.00	39.64
ATOM	5928	N	THR	746	53.783	2.001	34.224	1.00	37.50
ATOM	5930	CA	THR	746	55.066	2.462	33.728	1.00	37.56
ATOM	5931	CB	THR	746	56.108	2.571	34.869	1.00	38.58
ATOM	5932	OG1	THR	746	56.286	1.285	35.487	1.00	43.28
ATOM	5934	CG2	THR	746	55.666	3.567	35.899	1.00	34.64

ATOM	5935	C	THR	746	55.546	1.393	32.739	1.00	36.49
ATOM	5936	O	THR	746	55.118	0.234	32.817	1.00	34.18
ATOM	5937	N	PHE	747	56.453	1.768	31.839	1.00	35.27
ATOM	5939	CA	PHE	747	56.995	0.814	30.880	1.00	33.48
ATOM	5940	CB	PHE	747	58.025	1.475	29.970	1.00	34.35
ATOM	5941	CG	PHE	747	57.419	2.369	28.920	1.00	32.49
ATOM	5942	CD1	PHE	747	56.715	1.825	27.856	1.00	30.69
ATOM	5943	CD2	PHE	747	57.519	3.749	29.018	1.00	32.81
ATOM	5944	CE1	PHE	747	56.122	2.639	26.907	1.00	29.41
ATOM	5945	CE2	PHE	747	56.926	4.573	28.072	1.00	32.93
ATOM	5946	CZ	PHE	747	56.223	4.014	27.015	1.00	31.50
ATOM	5947	C	PHE	747	57.621	-0.363	31.606	1.00	34.65
ATOM	5948	O	PHE	747	57.616	-1.474	31.099	1.00	36.34
ATOM	5949	N	LYS	748	58.142	-0.128	32.808	1.00	37.75
ATOM	5951	CA	LYS	748	58.748	-1.205	33.583	1.00	39.67
ATOM	5952	CB	LYS	748	59.382	-0.664	34.873	1.00	43.06
ATOM	5953	CG	LYS	748	59.958	-1.757	35.774	1.00	48.96
ATOM	5954	CD	LYS	748	60.750	-1.207	36.966	1.00	52.20
ATOM	5955	CE	LYS	748	61.183	-2.344	37.907	1.00	53.62
ATOM	5956	NZ	LYS	748	62.057	-1.893	39.031	1.00	54.82
ATOM	5960	C	LYS	748	57.680	-2.263	33.882	1.00	39.65
ATOM	5961	O	LYS	748	57.902	-3.454	33.652	1.00	38.91
ATOM	5962	N	GLN	749	56.503	-1.818	34.331	1.00	39.39
ATOM	5964	CA	GLN	749	55.402	-2.742	34.623	1.00	40.70
ATOM	5965	CB	GLN	749	54.177	-1.991	35.140	1.00	43.82
ATOM	5966	CG	GLN	749	54.395	-1.149	36.373	1.00	50.97
ATOM	5967	CD	GLN	749	53.175	-0.304	36.715	1.00	55.53
ATOM	5968	OE1	GLN	749	53.272	0.914	36.895	1.00	55.80
ATOM	5969	NE2	GLN	749	52.012	-0.940	36.773	1.00	60.05
ATOM	5972	C	GLN	749	55.009	-3.455	33.334	1.00	40.03
ATOM	5973	O	GLN	749	54.903	-4.679	33.298	1.00	40.26
ATOM	5974	N	LEU	750	54.802	-2.666	32.278	1.00	39.18
ATOM	5976	CA	LEU	750	54.400	-3.171	30.964	1.00	36.65
ATOM	5977	CB	LEU	750	54.369	-2.039	29.927	1.00	34.58
ATOM	5978	CG	LEU	750	53.355	-0.910	30.116	1.00	32.52
ATOM	5979	CD1	LEU	750	53.644	0.210	29.125	1.00	31.67
ATOM	5980	CD2	LEU	750	51.947	-1.435	29.935	1.00	31.37
ATOM	5981	C	LEU	750	55.321	-4.255	30.477	1.00	35.81
ATOM	5982	O	LEU	750	54.856	-5.267	29.963	1.00	35.81
ATOM	5983	N	VAL	751	56.626	-4.035	30.620	1.00	37.38
ATOM	5985	CA	VAL	751	57.607	-5.029	30.193	1.00	38.66
ATOM	5986	CB	VAL	751	59.077	-4.545	30.411	1.00	35.42
ATOM	5987	CG1	VAL	751	60.075	-5.646	30.041	1.00	29.83
ATOM	5988	CG2	VAL	751	59.342	-3.324	29.559	1.00	29.95
ATOM	5989	C	VAL	751	57.337	-6.314	30.974	1.00	41.63
ATOM	5990	O	VAL	751	57.312	-7.401	30.396	1.00	42.43
ATOM	5991	N	GLU	752	57.051	-6.174	32.267	1.00	43.35
ATOM	5993	CA	GLU	752	56.766	-7.329	33.111	1.00	47.39
ATOM	5994	CB	GLU	752	56.674	-6.914	34.587	1.00	50.66
ATOM	5995	CG	GLU	752	57.950	-6.243	35.101	1.00	54.77
ATOM	5996	CD	GLU	752	58.006	-6.101	36.612	1.00	55.14
ATOM	5997	OE1	GLU	752	58.246	-4.972	37.102	1.00	54.14
ATOM	5998	OE2	GLU	752	57.844	-7.131	37.308	1.00	57.73
ATOM	5999	C	GLU	752	55.496	-8.068	32.655	1.00	46.00

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ATOM	6000	O	GLU	752	55.548	-9.261	32.328	1.00	46.25
ATOM	6001	N	ASP	753	54.380	-7.346	32.601	1.00	44.35
ATOM	6003	CA	ASP	753	53.099	-7.912	32.180	1.00	44.19
ATOM	6004	CB	ASP	753	52.059	-6.814	31.985	1.00	46.22
ATOM	6005	CG	ASP	753	51.512	-6.279	33.278	1.00	50.48
ATOM	6006	OD1	ASP	753	51.396	-7.062	34.248	1.00	52.15
ATOM	6007	OD2	ASP	753	51.170	-5.069	33.306	1.00	52.20
ATOM	6008	C	ASP	753	53.244	-8.608	30.849	1.00	44.54
ATOM	6009	O	ASP	753	52.770	-9.724	30.674	1.00	46.03
ATOM	6010	N	LEU	754	53.880	-7.918	29.906	1.00	44.43
ATOM	6012	CA	LEU	754	54.079	-8.438	28.563	1.00	43.70
ATOM	6013	CB	LEU	754	54.570	-7.339	27.618	1.00	43.48
ATOM	6014	CG	LEU	754	53.481	-6.350	27.201	1.00	44.67
ATOM	6015	CD1	LEU	754	54.095	-5.218	26.399	1.00	44.51
ATOM	6016	CD2	LEU	754	52.384	-7.069	26.408	1.00	42.07
ATOM	6017	C	LEU	754	54.993	-9.642	28.512	1.00	43.14
ATOM	6018	O	LEU	754	54.795	-10.536	27.697	1.00	41.32
ATOM	6019	N	ASP	755	55.990	-9.671	29.383	1.00	44.74
ATOM	6021	CA	ASP	755	56.897	-10.800	29.426	1.00	47.24
ATOM	6022	CB	ASP	755	57.942	-10.575	30.517	1.00	51.26
ATOM	6023	CG	ASP	755	59.121	-11.518	30.407	1.00	55.39
ATOM	6024	OD1	ASP	755	59.739	-11.793	31.455	1.00	60.61
ATOM	6025	OD2	ASP	755	59.443	-11.970	29.283	1.00	57.16
ATOM	6026	C	ASP	755	56.023	-12.005	29.771	1.00	47.67
ATOM	6027	O	ASP	755	56.041	-13.032	29.081	1.00	45.99
ATOM	6028	N	ARG	756	55.186	-11.816	30.789	1.00	46.72
ATOM	6030	CA	ARG	756	54.272	-12.851	31.256	1.00	46.25
ATOM	6031	CB	ARG	756	53.519	-12.368	32.499	1.00	46.31
ATOM	6032	CG	ARG	756	52.391	-13.287	32.953	1.00	46.99
ATOM	6033	CD	ARG	756	51.733	-12.776	34.227	1.00	48.10
ATOM	6034	NE	ARG	756	51.320	-11.379	34.118	1.00	53.67
ATOM	6036	CZ	ARG	756	50.294	-10.951	33.385	1.00	55.35
ATOM	6037	NH1	ARG	756	49.562	-11.812	32.684	1.00	54.10
ATOM	6040	NH2	ARG	756	50.008	-9.654	33.344	1.00	56.02
ATOM	6043	C	ARG	756	53.282	-13.261	30.175	1.00	45.05
ATOM	6044	O	ARG	756	53.213	-14.429	29.806	1.00	47.19
ATOM	6045	N	ILE	757	52.550	-12.289	29.647	1.00	43.47
ATOM	6047	CA	ILE	757	51.552	-12.553	28.617	1.00	43.80
ATOM	6048	CB	ILE	757	50.842	-11.241	28.161	1.00	42.02
ATOM	6049	CG2	ILE	757	49.811	-11.536	27.086	1.00	39.63
ATOM	6050	CG1	ILE	757	50.154	-10.578	29.361	1.00	40.00
ATOM	6051	CD1	ILE	757	49.600	-9.212	29.086	1.00	42.68
ATOM	6052	C	ILE	757	52.148	-13.296	27.428	1.00	46.03
ATOM	6053	O	ILE	757	51.549	-14.250	26.947	1.00	47.78
ATOM	6054	N	VAL	758	53.359	-12.925	27.015	1.00	49.03
ATOM	6056	CA	VAL	758	54.015	-13.584	25.884	1.00	51.51
ATOM	6057	CB	VAL	758	55.412	-12.971	25.556	1.00	50.75
ATOM	6058	CG1	VAL	758	56.105	-13.780	24.470	1.00	50.31
ATOM	6059	CG2	VAL	758	55.269	-11.541	25.081	1.00	52.52
ATOM	6060	C	VAL	758	54.209	-15.050	26.212	1.00	54.30
ATOM	6061	O	VAL	758	53.991	-15.915	25.369	1.00	54.80
ATOM	6062	N	ALA	759	54.617	-15.311	27.450	1.00	57.65
ATOM	6064	CA	ALA	759	54.858	-16.667	27.919	1.00	60.62
ATOM	6065	CB	ALA	759	55.423	-16.637	29.327	1.00	60.32

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ATOM	6066	C	ALA	759	53.571	-17.478	27.889	1.00	63.25	
ATOM	6067	O	ALA	759	53.568	-18.638	27.478	1.00	65.81	
ATOM	6068	N	LEU	760	52.475	-16.856	28.305	1.00	63.56	
ATOM	6070	CA	LEU	760	51.191	-17.533	28.333	1.00	64.25	
ATOM	6071	CB	LEU	760	50.302	-16.912	29.407	1.00	65.66	
ATOM	6072	CG	LEU	760	50.894	-16.962	30.820	1.00	65.62	
ATOM	6073	CD1	LEU	760	49.988	-16.246	31.809	1.00	64.75	
ATOM	6074	CD2	LEU	760	51.109	-18.410	31.227	1.00	66.65	
ATOM	6075	C	LEU	760	50.483	-17.535	26.984	1.00	64.89	
ATOM	6076	O	LEU	760	49.390	-18.088	26.860	1.00	66.37	
ATOM	6077	N	THR	761	51.103	-16.933	25.973	1.00	65.24	
ATOM	6079	CA	THR	761	50.516	-16.882	24.634	1.00	64.44	
ATOM	6080	CB	THR	761	50.829	-15.539	23.925	1.00	62.95	
ATOM	6081	OG1	THR	761	50.247	-14.463	24.669	1.00	62.70	
ATOM	6083	CG2	THR	761	50.249	-15.525	22.521	1.00	60.59	
ATOM	6084	C	THR	761	51.003	-18.044	23.769	1.00	64.71	
ATOM	6085	O	THR	761	52.202	-18.201	23.533	1.00	64.70	
ATOM	6086	SG	CYS	1603	18.536	-8.818	20.295	0.50	33.97	PRT2
ATOM	6087	CG	MET	534	69.178	12.159	22.968	0.50	31.30	PRT2
ATOM	6088	SD	MET	534	68.892	13.138	24.442	0.50	33.06	PRT2
ATOM	6089	CE	MET	534	70.060	12.456	25.568	0.50	34.22	PRT2
ATOM	6090	SG	CYS	603	56.041	-7.885	16.319	0.50	37.82	PRT2
ATOM	2682	OH2	TIP3	1	71.788	25.340	2.479	1.00	24.18	
ATOM	2685	OH2	TIP3	2	40.022	4.089	16.127	1.00	43.09	
ATOM	2688	OH2	TIP3	3	83.745	19.577	10.510	1.00	27.38	
ATOM	2691	OH2	TIP3	4	83.420	20.163	7.482	1.00	30.85	
ATOM	2694	OH2	TIP3	5	75.022	16.439	6.505	1.00	33.15	
ATOM	2697	OH2	TIP3	6	86.308	19.567	9.284	1.00	33.55	
ATOM	2700	OH2	TIP3	7	51.888	11.346	24.141	1.00	34.30	
ATOM	2703	OH2	TIP3	8	55.125	9.616	22.499	1.00	21.44	
ATOM	2706	OH2	TIP3	9	57.087	4.825	32.412	1.00	28.79	
ATOM	2709	OH2	TIP3	10	52.142	4.824	13.180	1.00	21.14	
ATOM	2712	OH2	TIP3	11	41.312	5.600	22.910	1.00	49.23	
ATOM	2715	OH2	TIP3	12	45.083	9.130	21.671	1.00	37.09	
ATOM	2718	OH2	TIP3	13	64.608	-2.335	28.803	1.00	44.31	
ATOM	2721	OH2	TIP3	14	77.192	13.199	23.753	1.00	32.96	
ATOM	2724	OH2	TIP3	15	79.201	17.296	17.997	1.00	38.51	
ATOM	2727	OH2	TIP3	16	82.988	11.608	15.745	1.00	27.56	
ATOM	2730	OH2	TIP3	17	14.096	-9.819	0.333	1.00	23.53	
ATOM	2733	OH2	TIP3	18	38.325	0.249	5.313	1.00	43.17	
ATOM	2736	OH2	TIP3	19	26.939	6.001	5.100	1.00	30.00	
ATOM	2739	OH2	TIP3	20	34.305	-1.615	16.992	1.00	44.82	
ATOM	2742	OH2	TIP3	21	20.300	2.328	27.798	1.00	45.23	
ATOM	2745	OH2	TIP3	22	50.996	-11.607	38.052	1.00	43.49	
ATOM	2748	OH2	TIP3	23	17.261	-6.167	-1.444	1.00	27.13	
ATOM	2751	OH2	TIP3	24	27.724	8.124	14.996	1.00	31.20	
ATOM	2754	OH2	TIP3	25	31.558	0.294	6.872	1.00	34.54	
ATOM	2757	OH2	TIP3	26	26.907	-12.815	28.161	1.00	49.20	
ATOM	2760	OH2	TIP3	27	28.705	-17.192	13.269	1.00	30.16	
ATOM	2763	OH2	TIP3	28	88.639	13.953	7.692	1.00	41.04	
ATOM	2766	OH2	TIP3	29	-2.328	-3.576	11.086	1.00	44.89	
ATOM	2769	OH2	TIP3	30	34.919	-4.069	19.070	1.00	53.72	
ATOM	2772	OH2	TIP3	31	80.124	17.865	9.324	1.00	28.96	
ATOM	2775	OH2	TIP3	32	5.417	3.492	10.771	1.00	34.07	

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ATOM	2778	OH2	TIP3	33	-10.718	4.889	11.542	1.00	30.81
ATOM	2781	OH2	TIP3	34	29.486	-8.823	20.599	1.00	51.35
ATOM	2784	OH2	TIP3	35	6.151	3.065	13.821	1.00	34.56
ATOM	2787	OH2	TIP3	36	31.907	2.919	0.361	1.00	48.13
ATOM	2790	OH2	TIP3	37	19.974	1.928	-3.873	1.00	30.12
ATOM	2793	OH2	TIP3	38	61.976	2.660	32.604	1.00	36.01
ATOM	2796	OH2	TIP3	39	21.084	-7.119	-3.759	1.00	20.12
ATOM	2799	OH2	TIP3	40	-15.729	8.693	22.468	1.00	54.88
ATOM	2802	OH2	TIP3	41	40.160	2.461	8.734	1.00	37.95
ATOM	2805	OH2	TIP3	42	19.248	11.349	0.190	1.00	37.63
ATOM	2808	OH2	TIP3	43	66.856	9.143	17.185	1.00	27.91
ATOM	2811	OH2	TIP3	44	87.262	19.150	18.734	1.00	57.83
ATOM	2814	OH2	TIP3	45	74.597	17.144	3.987	1.00	42.19
ATOM	2817	OH2	TIP3	46	29.192	16.988	10.582	1.00	37.28
ATOM	2820	OH2	TIP3	47	66.415	7.073	14.829	1.00	34.86
ATOM	2823	OH2	TIP3	48	85.063	21.453	5.510	1.00	27.42
ATOM	2826	OH2	TIP3	49	-4.716	2.835	2.998	1.00	40.54
ATOM	2829	OH2	TIP3	50	19.369	5.069	4.888	1.00	38.40
ATOM	2832	OH2	TIP3	51	34.750	5.517	24.999	1.00	29.11
ATOM	2835	OH2	TIP3	52	34.740	-16.765	14.093	1.00	32.68
ATOM	2838	OH2	TIP3	53	59.994	7.555	27.844	1.00	32.60
ATOM	2841	OH2	TIP3	54	-7.401	-1.595	6.080	1.00	43.73
ATOM	2844	OH2	TIP3	55	55.257	12.084	25.108	1.00	44.32
ATOM	2847	OH2	TIP3	56	68.239	6.953	16.647	1.00	44.46
ATOM	2850	OH2	TIP3	57	73.621	20.852	18.820	1.00	29.47
ATOM	2853	OH2	TIP3	58	3.399	-3.294	-8.210	1.00	22.31
ATOM	2856	OH2	TIP3	59	37.999	10.824	5.505	1.00	31.62
ATOM	2859	OH2	TIP3	60	29.779	-9.515	-1.395	1.00	40.76
ATOM	2862	OH2	TIP3	61	49.114	1.432	12.261	1.00	29.92
ATOM	2865	OH2	TIP3	62	41.257	4.012	29.005	1.00	39.24
ATOM	2868	OH2	TIP3	63	11.113	-12.848	1.296	1.00	34.36
ATOM	2871	OH2	TIP3	64	-1.221	-4.593	21.504	1.00	34.24
ATOM	2874	OH2	TIP3	65	30.002	16.453	13.258	1.00	49.66
ATOM	2877	OH2	TIP3	66	8.212	4.106	3.434	1.00	36.54
ATOM	2880	OH2	TIP3	67	72.868	18.807	22.589	1.00	38.26
ATOM	2883	OH2	TIP3	68	-8.056	-3.666	25.021	1.00	39.81
ATOM	2886	OH2	TIP3	69	66.436	-4.683	28.008	1.00	60.97
ATOM	2889	OH2	TIP3	70	22.063	-20.641	4.804	1.00	42.25
ATOM	2892	OH2	TIP3	71	59.860	-7.407	4.859	1.00	56.78
ATOM	2895	OH2	TIP3	72	16.887	-13.832	-2.611	1.00	59.32
ATOM	2898	OH2	TIP3	73	-15.108	7.351	4.303	1.00	31.87
ATOM	2901	OH2	TIP3	74	32.901	2.922	13.663	1.00	37.89
ATOM	2904	OH2	TIP3	75	0.173	-2.666	11.035	1.00	39.12
ATOM	2907	OH2	TIP3	76	17.533	2.317	5.808	1.00	18.66
ATOM	2910	OH2	TIP3	77	27.183	3.730	6.349	1.00	29.04
ATOM	2913	OH2	TIP3	78	-8.812	5.887	9.703	1.00	30.53
ATOM	2916	OH2	TIP3	79	1.614	-2.195	8.694	1.00	30.79
ATOM	2919	OH2	TIP3	80	-5.304	-3.157	6.846	1.00	47.38
ATOM	2922	OH2	TIP3	81	17.401	2.918	1.973	1.00	20.47
ATOM	2925	OH2	TIP3	82	20.333	3.188	3.159	1.00	24.44
ATOM	2928	OH2	TIP3	83	0.408	-2.516	22.276	1.00	31.11
ATOM	2931	OH2	TIP3	84	20.095	-6.123	-1.372	1.00	17.62
ATOM	2934	OH2	TIP3	85	11.018	-15.627	7.421	1.00	60.29
ATOM	2937	OH2	TIP3	86	4.089	-12.037	11.797	1.00	39.47

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ATOM	2940	OH2	TIP3 87	6.459	0.908	-3.278	1.00	30.31
ATOM	2943	OH2	TIP3 88	-13.493	1.004	5.319	1.00	41.13
ATOM	2946	OH2	TIP3 89	15.418	-7.532	0.022	1.00	21.29
ATOM	2949	OH2	TIP3 90	-2.128	-5.834	4.052	1.00	57.55
ATOM	2952	OH2	TIP3 91	12.731	4.833	-4.212	1.00	44.52
ATOM	2955	OH2	TIP3 92	69.320	27.812	2.191	1.00	37.47
ATOM	2958	OH2	TIP3 93	24.851	-12.871	0.285	1.00	44.73
ATOM	2961	OH2	TIP3 94	60.301	-4.459	33.927	1.00	40.13
ATOM	2964	OH2	TIP3 95	10.488	5.951	3.205	1.00	41.53
ATOM	2967	OH2	TIP3 96	-9.708	-4.233	4.439	1.00	29.77
ATOM	2970	OH2	TIP3 97	72.950	-1.768	10.144	1.00	39.69
ATOM	2973	OH2	TIP3 98	-3.287	5.612	30.618	1.00	34.65
ATOM	2976	OH2	TIP3 99	36.658	1.007	11.717	1.00	35.43
ATOM	2979	OH2	TIP3 100	21.221	6.459	16.863	1.00	20.70
ATOM	2982	OH2	TIP3 101	5.833	-8.726	22.274	1.00	47.13
ATOM	2985	OH2	TIP3 102	-13.529	7.868	17.445	1.00	31.95
ATOM	2988	OH2	TIP3 103	26.795	-10.682	-0.807	1.00	28.65
ATOM	2991	OH2	TIP3 104	23.711	1.909	18.309	1.00	28.29
ATOM	2994	OH2	TIP3 105	-2.187	12.232	3.920	1.00	44.98
ATOM	2997	OH2	TIP3 106	59.483	12.398	33.535	1.00	39.58
ATOM	3000	OH2	TIP3 107	4.439	-10.915	1.996	1.00	43.77
ATOM	3003	OH2	TIP3 108	8.041	2.687	0.648	1.00	45.32
ATOM	3006	OH2	TIP3 109	75.836	1.477	25.476	1.00	41.65
ATOM	3009	OH2	TIP3 110	48.604	15.594	14.349	1.00	36.36
ATOM	3012	OH2	TIP3 111	2.396	-11.387	9.259	1.00	34.21
ATOM	3015	OH2	TIP3 112	82.927	26.453	12.807	1.00	36.54
ATOM	3018	OH2	TIP3 113	8.983	-6.631	-3.299	1.00	47.01
ATOM	3021	OH2	TIP3 114	-8.690	4.367	4.504	1.00	41.25
ATOM	3024	OH2	TIP3 115	7.941	-13.921	8.777	1.00	36.12
ATOM	3027	OH2	TIP3 116	51.295	6.440	10.632	1.00	28.37
ATOM	3030	OH2	TIP3 117	20.432	3.771	15.637	1.00	31.22
ATOM	3033	OH2	TIP3 118	72.882	3.887	20.227	1.00	30.22
ATOM	3036	OH2	TIP3 119	5.187	-11.863	22.711	1.00	47.49
ATOM	3039	OH2	TIP3 120	33.889	2.571	16.293	1.00	40.04
ATOM	3042	OH2	TIP3 121	9.504	-12.183	7.160	1.00	31.48
ATOM	3045	OH2	TIP3 122	8.397	3.827	-1.647	1.00	46.92
ATOM	3048	OH2	TIP3 123	7.281	7.321	2.391	1.00	62.46
ATOM	3051	OH2	TIP3 124	35.682	-1.725	0.534	1.00	36.75
ATOM	3054	OH2	TIP3 125	44.465	10.095	11.089	1.00	44.72
ATOM	3057	OH2	TIP3 126	45.247	11.893	21.405	1.00	33.51
ATOM	3060	OH2	TIP3 127	57.386	-10.506	14.020	1.00	45.72
ATOM	3063	OH2	TIP3 128	-3.033	15.103	16.644	1.00	38.48
ATOM	3066	OH2	TIP3 129	85.621	11.111	8.814	1.00	38.13
ATOM	3069	OH2	TIP3 130	13.040	-2.760	2.176	1.00	31.26
ATOM	3072	OH2	TIP3 131	75.607	3.932	20.836	1.00	55.09
ATOM	3075	OH2	TIP3 132	13.080	7.467	-2.358	1.00	35.05
ATOM	3078	OH2	TIP3 133	11.308	-9.967	0.995	1.00	28.96
ATOM	3081	OH2	TIP3 134	13.716	-16.170	3.848	1.00	44.64
ATOM	3084	OH2	TIP3 135	-6.498	-3.706	16.178	1.00	43.17
ATOM	3087	OH2	TIP3 136	25.841	-12.949	3.950	1.00	41.14
ATOM	3090	OH2	TIP3 137	-16.285	10.803	6.585	1.00	45.75
ATOM	3093	OH2	TIP3 138	86.457	12.585	6.477	1.00	36.37
ATOM	3096	OH2	TIP3 139	32.097	-4.644	2.224	1.00	28.35
ATOM	3099	OH2	TIP3 140	44.936	7.528	11.961	1.00	46.60

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ATOM	3102	OH2	TIP3	141	80.781	12.162	16.353	1.00	41.46
ATOM	3105	OH2	TIP3	142	2.547	-7.532	-1.453	1.00	41.42
ATOM	3108	OH2	TIP3	143	31.850	-5.907	21.194	1.00	54.70
ATOM	3111	OH2	TIP3	144	74.524	-2.663	12.264	1.00	40.35
ATOM	3114	OH2	TIP3	145	7.592	6.769	-0.931	1.00	58.34
ATOM	3117	OH2	TIP3	146	71.168	5.735	21.648	1.00	27.86
ATOM	3120	OH2	TIP3	147	67.876	-4.900	8.725	1.00	33.58
ATOM	3123	OH2	TIP3	148	0.554	-10.181	6.605	1.00	75.65
ATOM	3126	OH2	TIP3	149	67.965	18.266	10.874	1.00	30.42
ATOM	3129	OH2	TIP3	150	3.509	8.125	4.021	1.00	40.77
ATOM	3132	OH2	TIP3	151	52.216	12.175	18.131	1.00	47.63
ATOM	3135	OH2	TIP3	152	-10.336	6.394	5.014	1.00	48.53
ATOM	3138	OH2	TIP3	153	76.427	1.384	-1.196	1.00	47.21
ATOM	3141	OH2	TIP3	154	10.116	-12.199	17.089	1.00	70.16
ATOM	3144	OH2	TIP3	155	34.043	14.595	18.314	1.00	40.56
ATOM	3147	OH2	TIP3	156	2.488	-8.304	16.835	1.00	64.47
ATOM	3150	OH2	TIP3	157	29.610	1.954	6.685	1.00	48.74
ATOM	3153	OH2	TIP3	158	32.578	-17.270	12.109	1.00	37.35
ATOM	3156	OH2	TIP3	159	42.013	18.106	11.196	1.00	68.33
ATOM	3159	OH2	TIP3	160	87.646	10.346	5.465	1.00	75.39
ATOM	3162	OH2	TIP3	161	69.931	-3.739	24.921	1.00	70.42
ATOM	3165	OH2	TIP3	162	77.277	5.700	23.531	1.00	53.26
ATOM	3168	OH2	TIP3	163	34.172	15.704	1.865	1.00	44.88
ATOM	3171	OH2	TIP3	164	-9.871	7.514	7.751	1.00	39.18
ATOM	3174	OH2	TIP3	165	11.814	5.604	7.443	1.00	46.70
ATOM	3177	OH2	TIP3	166	-8.801	13.912	13.532	1.00	52.89
ATOM	3180	OH2	TIP3	167	32.195	3.409	18.336	1.00	32.33
ATOM	3183	OH2	TIP3	168	-8.858	9.696	24.279	1.00	38.90
ATOM	3186	OH2	TIP3	169	-1.135	-6.924	15.691	1.00	43.05
ATOM	3189	OH2	TIP3	170	79.806	0.323	15.371	1.00	36.91
ATOM	3192	OH2	TIP3	171	67.181	20.622	-1.545	1.00	44.72
ATOM	3195	OH2	TIP3	172	-0.823	3.732	1.065	1.00	52.11
ATOM	3198	OH2	TIP3	173	-0.130	6.021	2.491	1.00	40.87
ATOM	3201	OH2	TIP3	174	-1.027	8.941	1.064	1.00	60.72
ATOM	3204	OH2	TIP3	175	-5.566	8.867	2.163	1.00	47.25
ATOM	3207	OH2	TIP3	176	-7.259	10.294	4.033	1.00	53.61
ATOM	3210	OH2	TIP3	177	2.664	7.247	1.058	1.00	46.41
ATOM	3213	OH2	TIP3	178	5.295	10.728	8.257	1.00	39.84
ATOM	3216	OH2	TIP3	179	63.743	12.726	22.713	1.00	49.55
ATOM	3219	OH2	TIP3	180	79.165	1.016	17.948	1.00	51.41
ATOM	3222	OH2	TIP3	181	13.823	-1.538	-3.942	1.00	39.85
ATOM	3225	OH2	TIP3	182	59.255	3.213	32.873	1.00	76.77
ATOM	3228	OH2	TIP3	183	32.210	13.612	20.027	1.00	60.41
ATOM	3231	OH2	TIP3	184	72.606	16.267	22.574	1.00	60.78
ATOM	3234	OH2	TIP3	185	-0.147	5.713	30.877	1.00	50.19
ATOM	3237	OH2	TIP3	186	-1.207	-4.507	27.969	1.00	65.19
ATOM	3240	OH2	TIP3	187	81.340	15.584	16.808	1.00	64.48
ATOM	3243	OH2	TIP3	188	-17.535	3.884	23.785	1.00	57.17
ATOM	3246	OH2	TIP3	189	27.503	10.697	14.669	1.00	36.11
ATOM	3249	OH2	TIP3	190	34.585	4.535	27.618	1.00	61.68
ATOM	3252	OH2	TIP3	191	-3.701	-4.982	9.069	1.00	43.66
ATOM	3255	OH2	TIP3	192	42.524	7.811	22.390	1.00	34.53
ATOM	3258	OH2	TIP3	193	52.937	11.764	21.790	1.00	36.19
ATOM	3261	OH2	TIP3	194	-7.665	8.600	6.358	1.00	59.08

ATOM	3264	OH2	TIP3	195	86.880	5.187	16.579	1.00	55.88
ATOM	3267	OH2	TIP3	196	55.377	16.147	20.540	1.00	48.25
ATOM	3270	OH2	TIP3	197	51.394	19.664	22.988	1.00	46.81
ATOM	3273	OH2	TIP3	198	20.021	7.087	7.226	1.00	52.98
ATOM	3276	OH2	TIP3	199	28.959	1.819	-3.219	1.00	40.50
ATOM	3279	OH2	TIP3	200	26.533	2.812	-4.295	1.00	54.24
ATOM	3282	OH2	TIP3	201	36.739	3.003	18.397	1.00	42.13
ATOM	3285	OH2	TIP3	202	16.968	-20.752	14.318	1.00	54.54
ATOM	3288	OH2	TIP3	203	28.177	-14.418	6.134	1.00	61.36
ATOM	3291	OH2	TIP3	204	31.488	1.501	-1.796	1.00	47.49
ATOM	3294	OH2	TIP3	205	10.665	-16.494	15.731	1.00	41.42
ATOM	3297	OH2	TIP3	206	6.916	-12.200	6.160	1.00	61.94
ATOM	3300	OH2	TIP3	207	-12.659	14.357	10.908	1.00	52.96
ATOM	3303	OH2	TIP3	208	11.274	9.662	-1.588	1.00	48.45
ATOM	3306	OH2	TIP3	209	11.491	12.484	-1.531	1.00	44.51
ATOM	3309	OH2	TIP3	210	34.037	13.520	-1.011	1.00	48.43
ATOM	3312	OH2	TIP3	211	31.162	18.259	7.980	1.00	44.86
ATOM	3315	OH2	TIP3	212	36.937	11.633	-1.971	1.00	49.85
ATOM	3318	OH2	TIP3	213	64.024	13.599	26.505	1.00	37.53
ATOM	3321	OH2	TIP3	214	36.528	5.933	14.857	1.00	57.04
ATOM	3324	OH2	TIP3	215	90.599	4.042	6.342	1.00	54.08
ATOM	3327	OH2	TIP3	216	50.139	-11.645	10.526	1.00	54.64
ATOM	3330	OH2	TIP3	217	66.523	-1.024	30.536	1.00	39.41
ATOM	3333	OH2	TIP3	218	74.880	18.976	20.591	1.00	41.84
ATOM	3336	OH2	TIP3	219	-3.095	9.744	3.142	1.00	52.35
ATOM	3339	OH2	TIP3	220	5.601	-3.682	25.022	1.00	29.30
ATOM	3342	OH2	TIP3	221	35.616	6.407	12.455	1.00	44.48
ATOM	3345	OH2	TIP3	222	-5.381	16.006	14.081	1.00	44.23
ATOM	3348	OH2	TIP3	223	46.509	-11.503	26.814	1.00	53.82
ATOM	3351	OH2	TIP3	224	-3.791	-5.481	20.929	1.00	61.42
ATOM	3354	OH2	TIP3	225	1.622	-3.876	-0.402	1.00	58.60
ATOM	3357	OH2	TIP3	226	86.244	11.220	23.133	1.00	59.84
ATOM	3360	OH2	TIP3	227	11.011	7.959	5.659	1.00	63.07
ATOM	3363	OH2	TIP3	228	64.610	-8.031	20.406	1.00	48.11
ATOM	3366	OH2	TIP3	229	11.446	-17.829	13.438	1.00	51.35
ATOM	3369	OH2	TIP3	230	72.056	1.258	-1.830	1.00	43.88
ATOM	3372	OH2	TIP3	231	57.359	9.732	11.744	1.00	65.45
ATOM	3375	OH2	TIP3	232	43.344	20.728	30.066	1.00	61.52
ATOM	3378	OH2	TIP3	233	66.723	16.772	15.661	1.00	43.79
ATOM	3381	OH2	TIP3	234	88.036	22.036	4.257	1.00	61.83
ATOM	3384	OH2	TIP3	235	12.085	2.346	27.862	1.00	46.29
ATOM	3387	OH2	TIP3	236	64.898	-0.425	3.209	1.00	50.06
ATOM	3390	OH2	TIP3	237	72.114	28.348	7.731	1.00	53.01
ATOM	3393	OH2	TIP3	238	25.792	-8.081	27.181	1.00	55.19
ATOM	3396	OH2	TIP3	239	-18.262	10.614	12.607	1.00	51.54
ATOM	3399	OH2	TIP3	240	30.336	11.280	16.201	1.00	46.53
ATOM	3402	OH2	TIP3	241	22.712	-15.818	-2.226	1.00	47.29
ATOM	3405	OH2	TIP3	242	29.700	9.496	18.074	1.00	40.10
ATOM	3408	OH2	TIP3	243	63.297	-0.480	5.497	1.00	49.90
ATOM	3411	OH2	TIP3	244	61.458	7.093	11.497	1.00	45.71
ATOM	3414	OH2	TIP3	245	-0.217	2.232	32.172	1.00	46.12
ATOM	3417	OH2	TIP3	246	66.196	6.250	12.159	1.00	34.47

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TABLE 3

Atom No.	Atom Type	A.A Type	A.A No.	X	Y	Z	OCC	B
ATOM	1	N	GLU	1464	-13.712	16.996	8.424	1.00 61.15
ATOM	3	CA	GLU	1464	-12.478	17.133	7.646	1.00 60.03
ATOM	4	CB	GLU	1464	-11.465	18.020	8.378	1.00 62.43
ATOM	5	C	GLU	1464	-11.865	15.766	7.319	1.00 57.36
ATOM	6	O	GLU	1464	-11.765	15.402	6.145	1.00 60.80
ATOM	7	N	LEU	1465	-11.466	15.003	8.333	1.00 50.25
ATOM	9	CA	LEU	1465	-10.899	13.691	8.067	1.00 42.73
ATOM	10	CB	LEU	1465	-10.097	13.171	9.258	1.00 41.34
ATOM	11	CG	LEU	1465	-8.571	13.277	9.169	1.00 39.78
ATOM	12	CD1	LEU	1465	-8.175	14.728	8.977	1.00 45.14
ATOM	13	CD2	LEU	1465	-7.926	12.722	10.426	1.00 34.20
ATOM	14	C	LEU	1465	-12.009	12.706	7.748	1.00 39.42
ATOM	15	O	LEU	1465	-13.070	12.719	8.375	1.00 36.63
ATOM	16	N	PRO	1466	-11.821	11.919	6.682	1.00 38.54
ATOM	17	CD	PRO	1466	-10.682	12.019	5.751	1.00 37.04
ATOM	18	CA	PRO	1466	-12.781	10.902	6.232	1.00 38.75
ATOM	19	CB	PRO	1466	-12.176	10.426	4.910	1.00 39.49
ATOM	20	CG	PRO	1466	-10.681	10.667	5.109	1.00 40.64
ATOM	21	C	PRO	1466	-12.859	9.756	7.246	1.00 39.08
ATOM	22	O	PRO	1466	-11.834	9.283	7.748	1.00 41.23
ATOM	23	N	GLU	1467	-14.064	9.278	7.513	1.00 37.11
ATOM	25	CA	GLU	1467	-14.247	8.213	8.482	1.00 35.96
ATOM	26	CB	GLU	1467	-15.725	8.123	8.863	1.00 39.90
ATOM	27	CG	GLU	1467	-16.334	9.410	9.417	1.00 46.64
ATOM	28	CD	GLU	1467	-17.823	9.280	9.694	1.00 51.50
ATOM	29	OE1	GLU	1467	-18.294	8.135	9.854	1.00 54.17
ATOM	30	OE2	GLU	1467	-18.529	10.315	9.756	1.00 53.39
ATOM	31	C	GLU	1467	-13.794	6.865	7.939	1.00 33.77
ATOM	32	O	GLU	1467	-13.885	6.632	6.740	1.00 36.27
ATOM	33	N	ASP	1468	-13.291	5.991	8.813	1.00 29.80
ATOM	35	CA	ASP	1468	-12.869	4.649	8.409	1.00 28.19
ATOM	36	CB	ASP	1468	-11.362	4.567	8.120	1.00 27.83
ATOM	37	CG	ASP	1468	-10.942	3.223	7.507	1.00 27.78
ATOM	38	OD1	ASP	1468	-11.689	2.225	7.592	1.00 25.64
ATOM	39	OD2	ASP	1468	-9.836	3.165	6.935	1.00 27.59
ATOM	40	C	ASP	1468	-13.244	3.672	9.512	1.00 28.05
ATOM	41	O	ASP	1468	-12.462	3.404	10.437	1.00 25.89
ATOM	42	N	PRO	1469	-14.446	3.089	9.403	1.00 29.07
ATOM	43	CD	PRO	1469	-15.401	3.311	8.298	1.00 29.93
ATOM	44	CA	PRO	1469	-14.981	2.124	10.365	1.00 28.65
ATOM	45	CB	PRO	1469	-16.235	1.615	9.659	1.00 30.89
ATOM	46	CG	PRO	1469	-16.690	2.811	8.879	1.00 28.99
ATOM	47	C	PRO	1469	-14.029	0.974	10.687	1.00 27.63
ATOM	48	O	PRO	1469	-14.136	0.364	11.748	1.00 26.94
ATOM	49	N	ARG	1470	-13.128	0.666	9.758	1.00 26.37
ATOM	51	CA	ARG	1470	-12.161	-0.414	9.947	1.00 26.64

ATOM	52	CB	ARG	1470	-11.363	-0.661	8.666	1.00	27.12
ATOM	53	CG	ARG	1470	-12.150	-1.014	7.424	1.00	29.72
ATOM	54	CD	ARG	1470	-11.189	-1.184	6.236	1.00	30.37
ATOM	55	NE	ARG	1470	-10.450	0.044	5.971	1.00	32.56
ATOM	57	CZ	ARG	1470	-9.624	0.211	4.948	1.00	37.69
ATOM	58	NH1	ARG	1470	-9.428	-0.784	4.091	1.00	44.25
ATOM	61	NH2	ARG	1470	-8.997	1.370	4.778	1.00	34.12
ATOM	64	C	ARG	1470	-11.129	-0.176	11.051	1.00	27.58
ATOM	65	O	ARG	1470	-10.504	-1.123	11.522	1.00	28.12
ATOM	66	N	TRP	1471	-10.900	1.079	11.421	1.00	27.62
ATOM	68	CA	TRP	1471	-9.870	1.362	12.408	1.00	26.66
ATOM	69	CB	TRP	1471	-8.661	1.938	11.686	1.00	24.95
ATOM	70	CG	TRP	1471	-8.010	0.951	10.790	1.00	25.65
ATOM	71	CD2	TRP	1471	-7.100	-0.083	11.186	1.00	23.19
ATOM	72	CE2	TRP	1471	-6.734	-0.776	10.022	1.00	21.80
ATOM	73	CE3	TRP	1471	-6.567	-0.489	12.414	1.00	21.84
ATOM	74	CD1	TRP	1471	-8.155	0.843	9.435	1.00	23.15
ATOM	75	NE1	TRP	1471	-7.388	-0.192	8.970	1.00	23.32
ATOM	77	CZ2	TRP	1471	-5.855	-1.857	10.052	1.00	22.54
ATOM	78	CZ3	TRP	1471	-5.698	-1.564	12.439	1.00	21.72
ATOM	79	CH2	TRP	1471	-5.352	-2.235	11.269	1.00	21.90
ATOM	80	C	TRP	1471	-10.224	2.278	13.558	1.00	28.44
ATOM	81	O	TRP	1471	-9.497	2.334	14.546	1.00	29.29
ATOM	82	N	GLU	1472	-11.317	3.015	13.424	1.00	29.49
ATOM	84	CA	GLU	1472	-11.719	3.962	14.453	1.00	29.97
ATOM	85	CB	GLU	1472	-12.920	4.769	13.961	1.00	33.80
ATOM	86	CG	GLU	1472	-13.218	6.050	14.731	1.00	33.27
ATOM	87	CD	GLU	1472	-12.475	7.249	14.195	1.00	34.26
ATOM	88	OE1	GLU	1472	-11.970	7.191	13.055	1.00	38.00
ATOM	89	OE2	GLU	1472	-12.413	8.265	14.910	1.00	34.01
ATOM	90	C	GLU	1472	-12.034	3.366	15.826	1.00	27.30
ATOM	91	O	GLU	1472	-12.640	2.309	15.945	1.00	28.36
ATOM	92	N	LEU	1473	-11.619	4.069	16.866	1.00	25.91
ATOM	94	CA	LEU	1473	-11.896	3.652	18.229	1.00	24.89
ATOM	95	CB	LEU	1473	-10.625	3.210	18.948	1.00	24.70
ATOM	96	CG	LEU	1473	-10.766	2.923	20.454	1.00	24.56
ATOM	97	CD1	LEU	1473	-11.498	1.613	20.701	1.00	21.89
ATOM	98	CD2	LEU	1473	-9.385	2.872	21.095	1.00	23.90
ATOM	99	C	LEU	1473	-12.426	4.907	18.882	1.00	27.05
ATOM	100	O	LEU	1473	-11.968	6.016	18.567	1.00	25.17
ATOM	101	N	PRO	1474	-13.479	4.766	19.706	1.00	28.20
ATOM	102	CD	PRO	1474	-14.290	3.551	19.886	1.00	29.92
ATOM	103	CA	PRO	1474	-14.088	5.897	20.411	1.00	30.61
ATOM	104	CB	PRO	1474	-15.197	5.224	21.226	1.00	28.15
ATOM	105	CG	PRO	1474	-15.613	4.110	20.357	1.00	24.28
ATOM	106	C	PRO	1474	-13.036	6.545	21.312	1.00	32.98
ATOM	107	O	PRO	1474	-12.253	5.838	21.968	1.00	34.79
ATOM	108	N	ARG	1475	-13.035	7.875	21.366	1.00	32.75
ATOM	110	CA	ARG	1475	-12.060	8.606	22.168	1.00	34.22
ATOM	111	CB	ARG	1475	-12.250	10.116	21.997	1.00	34.21
ATOM	112	CG	ARG	1475	-12.153	10.549	20.559	1.00	42.48
ATOM	113	CD	ARG	1475	-11.956	12.056	20.364	1.00	45.16

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ATOM	114	NE	ARG	1475	-11.655	12.317	18.954	1.00	45.65
ATOM	116	CZ	ARG	1475	-10.447	12.599	18.484	1.00	41.31
ATOM	117	NH1	ARG	1475	-9.420	12.686	19.318	1.00	35.94
ATOM	120	NH2	ARG	1475	-10.253	12.673	17.172	1.00	42.37
ATOM	123	C	ARG	1475	-12.114	8.232	23.641	1.00	35.29
ATOM	124	O	ARG	1475	-11.094	8.178	24.318	1.00	37.28
ATOM	125	N	ASP	1476	-13.304	7.931	24.129	1.00	35.37
ATOM	127	CA	ASP	1476	-13.468	7.570	25.526	1.00	36.97
ATOM	128	CB	ASP	1476	-14.952	7.586	25.896	1.00	39.47
ATOM	129	CG	ASP	1476	-15.748	6.501	25.205	1.00	40.02
ATOM	130	OD1	ASP	1476	-15.221	5.809	24.320	1.00	41.08
ATOM	131	OD2	ASP	1476	-16.926	6.327	25.571	1.00	47.00
ATOM	132	C	ASP	1476	-12.850	6.225	25.894	1.00	36.07
ATOM	133	O	ASP	1476	-12.830	5.842	27.066	1.00	36.26
ATOM	134	N	ARG	1477	-12.382	5.495	24.888	1.00	36.94
ATOM	136	CA	ARG	1477	-11.766	4.189	25.104	1.00	35.22
ATOM	137	CB	ARG	1477	-12.081	3.268	23.925	1.00	34.29
ATOM	138	CG	ARG	1477	-13.546	3.056	23.675	1.00	32.23
ATOM	139	CD	ARG	1477	-14.206	2.434	24.879	1.00	30.56
ATOM	140	NE	ARG	1477	-14.426	3.419	25.925	1.00	31.86
ATOM	142	CZ	ARG	1477	-14.730	3.126	27.182	1.00	33.09
ATOM	143	NH1	ARG	1477	-14.855	1.858	27.563	1.00	35.00
ATOM	146	NH2	ARG	1477	-14.904	4.101	28.053	1.00	29.62
ATOM	149	C	ARG	1477	-10.262	4.270	25.271	1.00	35.51
ATOM	150	O	ARG	1477	-9.621	3.290	25.637	1.00	36.44
ATOM	151	N	LEU	1478	-9.704	5.444	25.023	1.00	34.59
ATOM	153	CA	LEU	1478	-8.270	5.630	25.129	1.00	36.35
ATOM	154	CB	LEU	1478	-7.750	6.254	23.840	1.00	36.41
ATOM	155	CG	LEU	1478	-6.250	6.185	23.556	1.00	37.19
ATOM	156	CD1	LEU	1478	-5.791	4.728	23.479	1.00	34.63
ATOM	157	CD2	LEU	1478	-5.959	6.914	22.251	1.00	34.88
ATOM	158	C	LEU	1478	-7.901	6.517	26.325	1.00	38.74
ATOM	159	O	LEU	1478	-8.146	7.733	26.309	1.00	41.20
ATOM	160	N	VAL	1479	-7.311	5.907	27.355	1.00	36.92
ATOM	162	CA	VAL	1479	-6.885	6.622	28.560	1.00	35.79
ATOM	163	CB	VAL	1479	-6.929	5.693	29.780	1.00	35.81
ATOM	164	CG1	VAL	1479	-6.579	6.453	31.032	1.00	40.11
ATOM	165	CG2	VAL	1479	-8.302	5.056	29.907	1.00	35.59
ATOM	166	C	VAL	1479	-5.438	7.118	28.362	1.00	36.60
ATOM	167	O	VAL	1479	-4.479	6.369	28.583	1.00	33.48
ATOM	168	N	LEU	1480	-5.282	8.372	27.938	1.00	39.09
ATOM	170	CA	LEU	1480	-3.949	8.932	27.675	1.00	42.05
ATOM	171	CB	LEU	1480	-4.040	10.277	26.952	1.00	41.08
ATOM	172	CG	LEU	1480	-4.633	10.286	25.529	1.00	39.28
ATOM	173	CD1	LEU	1480	-4.766	11.720	25.051	1.00	40.04
ATOM	174	CD2	LEU	1480	-3.758	9.489	24.582	1.00	39.66
ATOM	175	C	LEU	1480	-3.001	9.027	28.867	1.00	41.51
ATOM	176	O	LEU	1480	-3.312	9.637	29.886	1.00	41.73
ATOM	177	N	GLY	1481	-1.817	8.444	28.697	1.00	40.68
ATOM	179	CA	GLY	1481	-0.849	8.439	29.775	1.00	41.28
ATOM	180	C	GLY	1481	0.412	9.225	29.529	1.00	43.08
ATOM	181	O	GLY	1481	0.474	10.147	28.701	1.00	45.65

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ATOM	182	N	LYS	1482	1.481	8.825	30.219	1.00	42.54
ATOM	184	CA	LYS	1482	2.781	9.453	30.128	1.00	43.74
ATOM	185	CB	LYS	1482	3.670	8.842	31.229	1.00	46.34
ATOM	186	CG	LYS	1482	5.155	8.979	30.954	1.00	52.23
ATOM	187	CD	LYS	1482	5.867	7.716	31.382	1.00	56.63
ATOM	188	CE	LYS	1482	5.373	6.518	30.607	1.00	54.20
ATOM	189	NZ	LYS	1482	6.199	5.320	30.955	1.00	59.97
ATOM	193	C	LYS	1482	3.552	9.422	28.806	1.00	43.96
ATOM	194	O	LYS	1482	3.557	8.422	28.111	1.00	44.68
ATOM	195	N	PRO	1483	4.259	10.521	28.481	1.00	44.06
ATOM	196	CD	PRO	1483	4.339	11.798	29.208	1.00	43.53
ATOM	197	CA	PRO	1483	5.005	10.573	27.208	1.00	44.07
ATOM	198	CB	PRO	1483	5.590	12.004	27.281	1.00	43.17
ATOM	199	CG	PRO	1483	4.630	12.738	28.114	1.00	43.75
ATOM	200	C	PRO	1483	6.172	9.543	27.116	1.00	43.47
ATOM	201	O	PRO	1483	6.853	9.308	28.120	1.00	43.76
ATOM	202	N	LEU	1484	6.408	9.001	25.932	1.00	41.71
ATOM	204	CA	LEU	1484	7.512	8.045	25.663	1.00	38.05
ATOM	205	CB	LEU	1484	6.964	6.803	24.927	1.00	33.38
ATOM	206	CG	LEU	1484	6.001	5.992	25.770	1.00	31.95
ATOM	207	CD1	LEU	1484	5.258	4.914	24.975	1.00	27.41
ATOM	208	CD2	LEU	1484	6.750	5.396	26.953	1.00	29.64
ATOM	209	C	LEU	1484	8.603	8.710	24.855	1.00	40.09
ATOM	210	O	LEU	1484	8.334	9.499	23.960	1.00	41.74
ATOM	211	N	GLY	1485	9.843	8.387	25.197	1.00	43.19
ATOM	213	CA	GLY	1485	10.976	8.923	24.512	1.00	50.32
ATOM	214	C	GLY	1485	11.261	10.408	24.697	1.00	54.65
ATOM	215	O	GLY	1485	11.036	10.973	25.770	1.00	54.73
ATOM	216	N	GLU	1486	11.747	11.072	23.647	1.00	59.07
ATOM	218	CA	GLU	1486	12.081	12.483	23.666	1.00	61.01
ATOM	219	CB	GLU	1486	13.489	12.646	24.275	1.00	62.51
ATOM	220	C	GLU	1486	12.014	13.183	22.295	1.00	62.48
ATOM	221	O	GLU	1486	12.901	13.970	21.949	1.00	64.10
ATOM	222	N	GLY	1487	10.975	12.892	21.519	1.00	62.29
ATOM	224	CA	GLY	1487	10.792	13.522	20.236	1.00	59.87
ATOM	225	C	GLY	1487	11.469	12.881	19.044	1.00	58.88
ATOM	226	O	GLY	1487	11.447	13.426	17.950	1.00	60.19
ATOM	227	N	ALA	1488	12.073	11.714	19.239	1.00	57.19
ATOM	229	CA	ALA	1488	12.721	11.016	18.140	1.00	55.59
ATOM	230	CB	ALA	1488	13.477	9.804	18.663	1.00	56.35
ATOM	231	C	ALA	1488	11.690	10.601	17.112	1.00	54.96
ATOM	232	O	ALA	1488	11.927	10.626	15.913	1.00	56.42
ATOM	233	N	PHE	1489	10.509	10.241	17.598	1.00	54.99
ATOM	235	CA	PHE	1489	9.401	9.807	16.721	1.00	54.07
ATOM	236	CB	PHE	1489	8.857	8.454	17.162	1.00	51.18
ATOM	237	CG	PHE	1489	9.880	7.373	17.137	1.00	46.81
ATOM	238	CD1	PHE	1489	10.641	7.093	18.271	1.00	46.81
ATOM	239	CD2	PHE	1489	10.096	6.612	15.984	1.00	48.30
ATOM	240	CE1	PHE	1489	11.585	6.090	18.262	1.00	47.41
ATOM	241	CE2	PHE	1489	11.040	5.601	15.963	1.00	48.23
ATOM	242	CZ	PHE	1489	11.794	5.336	17.111	1.00	47.94
ATOM	243	C	PHE	1489	8.261	10.814	16.748	1.00	54.90

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ATOM	244	O	PHE	1489	7.199	10.565	16.184	1.00	59.10
ATOM	245	N	GLY	1490	8.431	11.908	17.504	1.00	53.55
ATOM	247	CA	GLY	1490	7.432	12.958	17.611	1.00	50.20
ATOM	248	C	GLY	1490	6.745	12.844	18.942	1.00	49.82
ATOM	249	O	GLY	1490	7.266	12.161	19.837	1.00	50.95
ATOM	250	N	GLN	1491	5.614	13.514	19.124	1.00	49.53
ATOM	252	CA	GLN	1491	4.922	13.441	20.395	1.00	49.16
ATOM	253	CB	GLN	1491	3.927	14.590	20.564	1.00	51.74
ATOM	254	CG	GLN	1491	3.439	14.796	21.994	1.00	64.00
ATOM	255	CD	GLN	1491	2.545	16.039	22.180	1.00	71.35
ATOM	256	OE1	GLN	1491	2.534	16.922	21.352	1.00	77.94
ATOM	257	NE2	GLN	1491	1.824	16.083	23.289	1.00	76.51
ATOM	260	C	GLN	1491	4.207	12.083	20.505	1.00	45.94
ATOM	261	O	GLN	1491	3.151	11.869	19.919	1.00	48.02
ATOM	262	N	VAL	1492	4.848	11.129	21.184	1.00	41.00
ATOM	264	CA	VAL	1492	4.293	9.810	21.421	1.00	37.44
ATOM	265	CB	VAL	1492	5.235	8.665	21.025	1.00	34.74
ATOM	266	CG1	VAL	1492	4.593	7.325	21.285	1.00	28.97
ATOM	267	CG2	VAL	1492	5.632	8.769	19.553	1.00	35.78
ATOM	268	C	VAL	1492	4.014	9.621	22.901	1.00	38.67
ATOM	269	O	VAL	1492	4.907	9.769	23.735	1.00	38.62
ATOM	270	N	VAL	1493	2.776	9.276	23.250	1.00	39.98
ATOM	272	CA	VAL	1493	2.423	9.062	24.653	1.00	37.79
ATOM	273	CB	VAL	1493	1.257	9.970	25.093	1.00	37.36
ATOM	274	CG1	VAL	1493	1.489	11.403	24.689	1.00	39.11
ATOM	275	CG2	VAL	1493	-0.074	9.480	24.555	1.00	38.99
ATOM	276	C	VAL	1493	2.052	7.603	24.877	1.00	36.38
ATOM	277	O	VAL	1493	1.759	6.874	23.945	1.00	37.73
ATOM	278	N	LEU	1494	2.094	7.176	26.123	1.00	35.42
ATOM	280	CA	LEU	1494	1.718	5.817	26.483	1.00	33.65
ATOM	281	CB	LEU	1494	2.536	5.291	27.670	1.00	29.88
ATOM	282	CG	LEU	1494	2.117	3.945	28.279	1.00	30.31
ATOM	283	CD1	LEU	1494	2.103	2.844	27.244	1.00	30.83
ATOM	284	CD2	LEU	1494	3.049	3.574	29.400	1.00	32.12
ATOM	285	C	LEU	1494	0.260	5.934	26.870	1.00	34.27
ATOM	286	O	LEU	1494	-0.168	6.994	27.348	1.00	34.85
ATOM	287	N	ALA	1495	-0.527	4.898	26.608	1.00	32.20
ATOM	289	CA	ALA	1495	-1.930	4.954	26.980	1.00	29.71
ATOM	290	CB	ALA	1495	-2.724	5.722	25.930	1.00	25.48
ATOM	291	C	ALA	1495	-2.499	3.567	27.183	1.00	28.85
ATOM	292	O	ALA	1495	-1.826	2.563	26.998	1.00	27.28
ATOM	293	N	GLU	1496	-3.743	3.519	27.615	1.00	32.20
ATOM	295	CA	GLU	1496	-4.413	2.250	27.824	1.00	33.34
ATOM	296	CB	GLU	1496	-4.735	2.063	29.301	1.00	35.65
ATOM	297	CG	GLU	1496	-3.521	1.962	30.198	1.00	39.14
ATOM	298	CD	GLU	1496	-3.899	2.045	31.663	1.00	42.57
ATOM	299	OE1	GLU	1496	-4.469	3.083	32.061	1.00	42.59
ATOM	300	OE2	GLU	1496	-3.646	1.069	32.407	1.00	42.76
ATOM	301	C	GLU	1496	-5.692	2.274	26.994	1.00	33.40
ATOM	302	O	GLU	1496	-6.439	3.261	27.017	1.00	34.36
ATOM	303	N	ALA	1497	-5.875	1.247	26.177	1.00	31.67
ATOM	305	CA	ALA	1497	-7.051	1.168	25.351	1.00	31.23

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ATOM	306	CB	ALA	1497	-6.671	0.750	23.953	1.00	28.13
ATOM	307	C	ALA	1497	-8.000	0.168	25.974	1.00	32.02
ATOM	308	O	ALA	1497	-7.599	-0.954	26.261	1.00	33.45
ATOM	309	N	ILE	1498	-9.218	0.602	26.282	1.00	34.15
ATOM	311	CA	ILE	1498	-10.222	-0.294	26.854	1.00	35.89
ATOM	312	CB	ILE	1498	-11.294	0.453	27.679	1.00	35.30
ATOM	313	CG2	ILE	1498	-12.267	-0.551	28.300	1.00	32.95
ATOM	314	CG1	ILE	1498	-10.663	1.316	28.770	1.00	35.29
ATOM	315	CD1	ILE	1498	-11.656	2.262	29.419	1.00	31.69
ATOM	316	C	ILE	1498	-10.953	-0.929	25.680	1.00	38.79
ATOM	317	O	ILE	1498	-11.571	-0.227	24.877	1.00	37.46
ATOM	318	N	GLY	1499	-10.859	-2.245	25.559	1.00	43.14
ATOM	320	CA	GLY	1499	-11.544	-2.918	24.477	1.00	46.90
ATOM	321	C	GLY	1499	-10.673	-3.299	23.298	1.00	49.69
ATOM	322	O	GLY	1499	-9.921	-4.269	23.387	1.00	51.47
ATOM	323	N	LEU	1500	-10.739	-2.508	22.223	1.00	49.92
ATOM	325	CA	LEU	1500	-10.003	-2.765	20.973	1.00	49.62
ATOM	326	CB	LEU	1500	-8.478	-2.898	21.185	1.00	49.96
ATOM	327	CG	LEU	1500	-7.504	-1.703	21.167	1.00	49.26
ATOM	328	CD1	LEU	1500	-6.069	-2.217	21.284	1.00	47.17
ATOM	329	CD2	LEU	1500	-7.638	-0.883	19.899	1.00	47.80
ATOM	330	C	LEU	1500	-10.535	-4.027	20.275	1.00	49.49
ATOM	331	O	LEU	1500	-10.480	-5.145	20.806	1.00	47.99
ATOM	332	N	PRO	1505	-13.253	-5.837	25.284	1.00	50.58
ATOM	333	CD	PRO	1505	-13.877	-7.173	25.239	1.00	51.43
ATOM	334	CA	PRO	1505	-14.197	-4.825	25.779	1.00	48.08
ATOM	335	CB	PRO	1505	-15.548	-5.521	25.627	1.00	48.59
ATOM	336	CG	PRO	1505	-15.216	-6.944	25.940	1.00	51.66
ATOM	337	C	PRO	1505	-13.904	-4.396	27.227	1.00	44.58
ATOM	338	O	PRO	1505	-13.883	-3.202	27.531	1.00	42.73
ATOM	339	N	ASN	1506	-13.640	-5.363	28.102	1.00	42.10
ATOM	341	CA	ASN	1506	-13.337	-5.053	29.497	1.00	45.05
ATOM	342	CB	ASN	1506	-14.202	-5.893	30.434	1.00	47.04
ATOM	343	CG	ASN	1506	-15.657	-5.493	30.395	1.00	48.72
ATOM	344	OD1	ASN	1506	-15.999	-4.309	30.487	1.00	50.48
ATOM	345	ND2	ASN	1506	-16.529	-6.478	30.260	1.00	51.15
ATOM	348	C	ASN	1506	-11.863	-5.251	29.836	1.00	46.50
ATOM	349	O	ASN	1506	-11.487	-5.343	31.008	1.00	46.50
ATOM	350	N	ARG	1507	-11.029	-5.284	28.806	1.00	46.99
ATOM	352	CA	ARG	1507	-9.594	-5.466	28.976	1.00	47.52
ATOM	353	CB	ARG	1507	-9.111	-6.650	28.142	1.00	54.20
ATOM	354	CG	ARG	1507	-9.327	-7.993	28.781	1.00	64.52
ATOM	355	CD	ARG	1507	-8.402	-8.180	29.963	1.00	71.17
ATOM	356	NE	ARG	1507	-8.592	-9.494	30.556	1.00	76.52
ATOM	358	CZ	ARG	1507	-8.030	-9.898	31.689	1.00	81.64
ATOM	359	NH1	ARG	1507	-7.219	-9.096	32.375	1.00	83.30
ATOM	362	NH2	ARG	1507	-8.340	-11.093	32.174	1.00	84.44
ATOM	365	C	ARG	1507	-8.871	-4.234	28.485	1.00	43.46
ATOM	366	O	ARG	1507	-9.227	-3.695	27.440	1.00	42.73
ATOM	367	N	VAL	1508	-7.912	-3.749	29.265	1.00	40.84
ATOM	369	CA	VAL	1508	-7.143	-2.598	28.830	1.00	38.27
ATOM	370	CB	VAL	1508	-6.786	-1.604	29.961	1.00	34.90

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ATOM	371	CG1	VAL	1508	-8.038	-1.124	30.646	1.00	41.81
ATOM	372	CG2	VAL	1508	-5.850	-2.226	30.944	1.00	35.89
ATOM	373	C	VAL	1508	-5.874	-3.147	28.211	1.00	36.81
ATOM	374	O	VAL	1508	-5.371	-4.191	28.637	1.00	35.13
ATOM	375	N	THR	1509	-5.393	-2.465	27.180	1.00	36.04
ATOM	377	CA	THR	1509	-4.184	-2.854	26.485	1.00	33.31
ATOM	378	CB	THR	1509	-4.503	-3.254	25.025	1.00	33.79
ATOM	379	OG1	THR	1509	-5.511	-4.275	25.014	1.00	33.98
ATOM	381	CG2	THR	1509	-3.259	-3.774	24.321	1.00	32.78
ATOM	382	C	THR	1509	-3.268	-1.627	26.453	1.00	32.37
ATOM	383	O	THR	1509	-3.718	-0.533	26.113	1.00	31.97
ATOM	384	N	LYS	1510	-2.015	-1.786	26.884	1.00	32.96
ATOM	386	CA	LYS	1510	-1.071	-0.673	26.828	1.00	33.25
ATOM	387	CB	LYS	1510	0.157	-0.902	27.699	1.00	34.65
ATOM	388	CG	LYS	1510	-0.093	-0.909	29.197	1.00	39.64
ATOM	389	CD	LYS	1510	1.237	-1.105	29.913	1.00	43.51
ATOM	390	CE	LYS	1510	1.110	-1.949	31.173	1.00	48.42
ATOM	391	NZ	LYS	1510	0.399	-1.256	32.287	1.00	53.03
ATOM	395	C	LYS	1510	-0.646	-0.550	25.370	1.00	32.26
ATOM	396	O	LYS	1510	-0.240	-1.533	24.736	1.00	30.20
ATOM	397	N	VAL	1511	-0.760	0.665	24.849	1.00	32.28
ATOM	399	CA	VAL	1511	-0.436	0.980	23.472	1.00	30.73
ATOM	400	CB	VAL	1511	-1.738	1.140	22.666	1.00	32.25
ATOM	401	CG1	VAL	1511	-2.566	-0.147	22.723	1.00	29.00
ATOM	402	CG2	VAL	1511	-2.549	2.347	23.193	1.00	29.17
ATOM	403	C	VAL	1511	0.329	2.307	23.423	1.00	30.91
ATOM	404	O	VAL	1511	0.445	3.008	24.433	1.00	31.94
ATOM	405	N	ALA	1512	0.842	2.658	22.250	1.00	27.30
ATOM	407	CA	ALA	1512	1.550	3.914	22.094	1.00	24.22
ATOM	408	CB	ALA	1512	2.921	3.694	21.493	1.00	23.39
ATOM	409	C	ALA	1512	0.698	4.769	21.181	1.00	23.62
ATOM	410	O	ALA	1512	0.116	4.271	20.228	1.00	22.69
ATOM	411	N	VAL	1513	0.605	6.054	21.484	1.00	27.51
ATOM	413	CA	VAL	1513	-0.192	6.984	20.688	1.00	30.03
ATOM	414	CB	VAL	1513	-1.359	7.613	21.522	1.00	28.31
ATOM	415	CG1	VAL	1513	-2.218	8.522	20.650	1.00	28.93
ATOM	416	CG2	VAL	1513	-2.214	6.542	22.159	1.00	26.00
ATOM	417	C	VAL	1513	0.674	8.108	20.107	1.00	31.21
ATOM	418	O	VAL	1513	1.370	8.816	20.834	1.00	29.73
ATOM	419	N	LYS	1514	0.631	8.225	18.784	1.00	33.99
ATOM	421	CA	LYS	1514	1.342	9.258	18.037	1.00	35.44
ATOM	422	CB	LYS	1514	1.831	8.692	16.707	1.00	34.55
ATOM	423	CG	LYS	1514	2.835	7.586	16.872	1.00	35.38
ATOM	424	CD	LYS	1514	3.025	6.807	15.599	1.00	36.87
ATOM	425	CE	LYS	1514	3.457	7.710	14.438	1.00	45.19
ATOM	426	NZ	LYS	1514	4.598	8.622	14.755	1.00	44.31
ATOM	430	C	LYS	1514	0.304	10.345	17.761	1.00	35.97
ATOM	431	O	LYS	1514	-0.806	10.037	17.299	1.00	34.39
ATOM	432	N	MET	1515	0.673	11.596	18.028	1.00	38.17
ATOM	434	CA	MET	1515	-0.207	12.747	17.835	1.00	41.17
ATOM	435	CB	MET	1515	-0.901	13.098	19.145	1.00	39.54
ATOM	436	CG	MET	1515	0.075	13.428	20.255	1.00	39.11

ATOM	437	SD	MET	1515	-0.766	13.612	21.799	1.00	43.85
ATOM	438	CE	MET	1515	-1.212	11.937	22.087	1.00	46.18
ATOM	439	C	MET	1515	0.612	13.939	17.391	1.00	43.65
ATOM	440	O	MET	1515	1.834	13.905	17.445	1.00	45.72
ATOM	441	N	LEU	1516	-0.053	14.962	16.872	1.00	48.73
ATOM	443	CA	LEU	1516	0.640	16.175	16.448	1.00	52.23
ATOM	444	CB	LEU	1516	-0.152	16.917	15.374	1.00	49.77
ATOM	445	CG	LEU	1516	-0.413	16.254	14.036	1.00	48.04
ATOM	446	CD1	LEU	1516	-1.418	17.104	13.285	1.00	48.16
ATOM	447	CD2	LEU	1516	0.884	16.102	13.265	1.00	42.80
ATOM	448	C	LEU	1516	0.810	17.119	17.631	1.00	55.67
ATOM	449	O	LEU	1516	0.217	16.927	18.703	1.00	53.99
ATOM	450	N	LYS	1517	1.580	18.174	17.402	1.00	60.97
ATOM	452	CA	LYS	1517	1.823	19.193	18.416	1.00	65.19
ATOM	453	CB	LYS	1517	3.274	19.668	18.344	1.00	69.34
ATOM	454	CG	LYS	1517	4.294	18.559	18.529	1.00	72.86
ATOM	455	CD	LYS	1517	5.646	18.935	17.929	1.00	74.91
ATOM	456	CE	LYS	1517	6.686	17.851	18.197	1.00	74.38
ATOM	457	NZ	LYS	1517	8.010	18.241	17.649	1.00	75.45
ATOM	461	C	LYS	1517	0.879	20.357	18.139	1.00	65.97
ATOM	462	O	LYS	1517	0.303	20.451	17.053	1.00	64.59
ATOM	463	N	SER	1518	0.776	21.270	19.098	1.00	68.20
ATOM	465	CA	SER	1518	-0.107	22.422	18.972	1.00	71.92
ATOM	466	CB	SER	1518	-0.002	23.322	20.202	1.00	69.89
ATOM	467	C	SER	1518	0.144	23.247	17.718	1.00	74.68
ATOM	468	O	SER	1518	-0.798	23.604	17.006	1.00	77.44
ATOM	469	N	ASP	1519	1.417	23.493	17.422	1.00	76.04
ATOM	471	CA	ASP	1519	1.799	24.299	16.264	1.00	76.48
ATOM	472	CB	ASP	1519	3.126	25.011	16.539	1.00	77.59
ATOM	473	C	ASP	1519	1.912	23.525	14.958	1.00	75.88
ATOM	474	O	ASP	1519	2.374	24.075	13.959	1.00	77.52
ATOM	475	N	ALA	1520	1.486	22.265	14.956	1.00	74.39
ATOM	477	CA	ALA	1520	1.574	21.439	13.758	1.00	72.83
ATOM	478	CB	ALA	1520	0.930	20.079	14.010	1.00	73.06
ATOM	479	C	ALA	1520	0.889	22.153	12.598	1.00	71.47
ATOM	480	O	ALA	1520	-0.096	22.858	12.797	1.00	73.48
ATOM	481	N	THR	1521	1.440	22.015	11.401	1.00	69.15
ATOM	483	CA	THR	1521	0.858	22.653	10.234	1.00	70.05
ATOM	484	CB	THR	1521	1.950	23.110	9.272	1.00	70.21
ATOM	485	OG1	THR	1521	2.505	21.969	8.607	1.00	72.71
ATOM	487	CG2	THR	1521	3.053	23.815	10.043	1.00	71.01
ATOM	488	C	THR	1521	-0.015	21.616	9.550	1.00	70.64
ATOM	489	O	THR	1521	0.015	20.443	9.932	1.00	72.38
ATOM	490	N	GLU	1522	-0.782	22.026	8.542	1.00	69.70
ATOM	492	CA	GLU	1522	-1.623	21.081	7.815	1.00	67.41
ATOM	493	CB	GLU	1522	-2.478	21.800	6.761	1.00	70.01
ATOM	494	C	GLU	1522	-0.718	20.024	7.168	1.00	64.50
ATOM	495	O	GLU	1522	-1.125	18.878	7.006	1.00	63.76
ATOM	496	N	LYS	1523	0.512	20.419	6.827	1.00	60.75
ATOM	498	CA	LYS	1523	1.483	19.502	6.240	1.00	58.57
ATOM	499	CB	LYS	1523	2.782	20.230	5.883	1.00	60.63
ATOM	500	CG	LYS	1523	3.909	19.318	5.361	1.00	62.47

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ATOM	501	CD	LYS	1523	3.459	18.461	4.168	1.00	63.35
ATOM	502	CE	LYS	1523	4.633	17.700	3.559	1.00	66.57
ATOM	503	NZ	LYS	1523	4.210	16.733	2.498	1.00	69.56
ATOM	507	C	LYS	1523	1.763	18.441	7.281	1.00	55.98
ATOM	508	O	LYS	1523	1.790	17.251	6.972	1.00	56.37
ATOM	509	N	ASP	1524	1.960	18.885	8.517	1.00	52.16
ATOM	511	CA	ASP	1524	2.211	17.980	9.630	1.00	48.91
ATOM	512	CB	ASP	1524	2.487	18.762	10.915	1.00	50.87
ATOM	513	CG	ASP	1524	3.865	19.401	10.928	1.00	53.00
ATOM	514	OD1	ASP	1524	4.004	20.511	11.489	1.00	53.77
ATOM	515	OD2	ASP	1524	4.816	18.785	10.394	1.00	56.30
ATOM	516	C	ASP	1524	1.032	17.031	9.831	1.00	45.34
ATOM	517	O	ASP	1524	1.221	15.858	10.176	1.00	45.63
ATOM	518	N	LEU	1525	-0.176	17.530	9.593	1.00	40.15
ATOM	520	CA	LEU	1525	-1.368	16.715	9.711	1.00	39.38
ATOM	521	CB	LEU	1525	-2.624	17.588	9.633	1.00	41.66
ATOM	522	CG	LEU	1525	-4.020	16.937	9.585	1.00	42.75
ATOM	523	CD1	LEU	1525	-4.245	15.945	10.727	1.00	42.97
ATOM	524	CD2	LEU	1525	-5.058	18.026	9.644	1.00	42.24
ATOM	525	C	LEU	1525	-1.340	15.699	8.575	1.00	39.77
ATOM	526	O	LEU	1525	-1.509	14.506	8.813	1.00	39.11
ATOM	527	N	SER	1526	-1.062	16.172	7.361	1.00	39.64
ATOM	529	CA	SER	1526	-0.998	15.320	6.181	1.00	40.65
ATOM	530	CB	SER	1526	-0.541	16.105	4.947	1.00	43.32
ATOM	531	OG	SER	1526	-1.398	17.190	4.656	1.00	52.41
ATOM	533	C	SER	1526	-0.015	14.201	6.383	1.00	39.12
ATOM	534	O	SER	1526	-0.346	13.038	6.198	1.00	41.75
ATOM	535	N	ASP	1527	1.203	14.553	6.769	1.00	38.30
ATOM	537	CA	ASP	1527	2.244	13.552	6.969	1.00	39.28
ATOM	538	CB	ASP	1527	3.531	14.208	7.471	1.00	41.16
ATOM	539	CG	ASP	1527	4.218	15.069	6.404	1.00	45.20
ATOM	540	OD1	ASP	1527	3.861	14.972	5.198	1.00	43.25
ATOM	541	OD2	ASP	1527	5.132	15.840	6.788	1.00	45.93
ATOM	542	C	ASP	1527	1.788	12.443	7.903	1.00	37.34
ATOM	543	O	ASP	1527	1.867	11.259	7.557	1.00	37.24
ATOM	544	N	LEU	1528	1.224	12.935	9.036	1.00	35.88
ATOM	546	CA	LEU	1528	0.728	11.874	10.009	1.00	35.07
ATOM	547	CB	LEU	1528	0.185	12.606	11.242	1.00	34.38
ATOM	548	CG	LEU	1528	-0.146	11.789	12.491	1.00	35.86
ATOM	549	CD1	LEU	1528	1.009	10.845	12.820	1.00	34.83
ATOM	550	CD2	LEU	1528	-0.435	12.711	13.642	1.00	29.98
ATOM	551	C	LEU	1528	-0.351	10.977	9.374	1.00	33.31
ATOM	552	O	LEU	1528	-0.342	9.756	9.552	1.00	34.55
ATOM	553	N	ILE	1529	-1.236	11.575	8.585	1.00	32.16
ATOM	555	CA	ILE	1529	-2.306	10.829	7.924	1.00	30.94
ATOM	556	CB	ILE	1529	-3.304	11.757	7.178	1.00	27.07
ATOM	557	CG2	ILE	1529	-4.388	10.926	6.521	1.00	26.06
ATOM	558	CG1	ILE	1529	-3.953	12.723	8.169	1.00	23.67
ATOM	559	CD1	ILE	1529	-4.877	13.736	7.526	1.00	22.34
ATOM	560	C	ILE	1529	-1.684	9.856	6.947	1.00	31.34
ATOM	561	O	ILE	1529	-2.058	8.683	6.912	1.00	33.57
ATOM	562	N	SER	1530	-0.703	10.331	6.191	1.00	30.74

ATOM	564	CA	SER	1530	0.007	9.496	5.230	1.00	32.04
ATOM	565	CB	SER	1530	1.109	10.302	4.548	1.00	35.20
ATOM	566	OG	SER	1530	0.596	11.501	4.002	1.00	41.97
ATOM	568	C	SER	1530	0.620	8.262	5.895	1.00	29.06
ATOM	569	O	SER	1530	0.478	7.140	5.377	1.00	26.64
ATOM	570	N	GLU	1531	1.287	8.464	7.034	1.00	23.86
ATOM	572	CA	GLU	1531	1.918	7.367	7.759	1.00	23.86
ATOM	573	CB	GLU	1531	2.729	7.893	8.944	1.00	25.69
ATOM	574	CG	GLU	1531	3.501	6.803	9.701	1.00	23.65
ATOM	575	CD	GLU	1531	4.341	7.319	10.868	1.00	26.03
ATOM	576	OE1	GLU	1531	4.927	6.473	11.572	1.00	25.92
ATOM	577	OE2	GLU	1531	4.435	8.549	11.094	1.00	26.55
ATOM	578	C	GLU	1531	0.906	6.325	8.222	1.00	25.44
ATOM	579	O	GLU	1531	1.200	5.126	8.228	1.00	23.67
ATOM	580	N	MET	1532	-0.285	6.788	8.600	1.00	26.39
ATOM	582	CA	MET	1532	-1.365	5.898	9.048	1.00	26.57
ATOM	583	CB	MET	1532	-2.473	6.720	9.714	1.00	24.81
ATOM	584	CG	MET	1532	-3.645	5.889	10.191	1.00	27.47
ATOM	585	SD	MET	1532	-4.969	6.899	10.860	1.00	28.43
ATOM	586	CE	MET	1532	-5.178	8.102	9.576	1.00	24.45
ATOM	587	C	MET	1532	-1.923	5.076	7.861	1.00	28.30
ATOM	588	O	MET	1532	-2.048	3.850	7.933	1.00	27.95
ATOM	589	N	GLU	1533	-2.221	5.760	6.762	1.00	28.95
ATOM	591	CA	GLU	1533	-2.732	5.111	5.565	1.00	30.32
ATOM	592	CB	GLU	1533	-2.983	6.143	4.476	1.00	25.40
ATOM	593	CG	GLU	1533	-4.064	7.127	4.852	1.00	26.09
ATOM	594	CD	GLU	1533	-5.402	6.461	5.119	1.00	25.89
ATOM	595	OE1	GLU	1533	-5.913	5.745	4.240	1.00	27.24
ATOM	596	OE2	GLU	1533	-5.964	6.662	6.209	1.00	30.00
ATOM	597	C	GLU	1533	-1.723	4.089	5.093	1.00	31.64
ATOM	598	O	GLU	1533	-2.080	2.983	4.706	1.00	33.57
ATOM	599	N	MET	1534	-0.455	4.472	5.166	1.00	33.57
ATOM	601	CA	MET	1534	0.664	3.618	4.793	1.00	32.86
ATOM	602	CB	MET	1534	1.957	4.390	5.003	1.00	32.89
ATOM	603	CG	MET	1534	3.159	3.559	4.851	1.00	39.27
ATOM	604	SD	MET	1534	3.577	3.513	3.164	1.00	51.24
ATOM	605	CE	MET	1534	5.153	4.319	3.204	1.00	44.97
ATOM	606	C	MET	1534	0.670	2.373	5.681	1.00	31.84
ATOM	607	O	MET	1534	0.816	1.250	5.198	1.00	33.78
ATOM	608	N	MET	1535	0.509	2.571	6.982	1.00	30.36
ATOM	610	CA	MET	1535	0.469	1.453	7.902	1.00	28.83
ATOM	611	CB	MET	1535	0.419	1.946	9.352	1.00	24.75
ATOM	612	CG	MET	1535	1.717	2.540	9.850	1.00	21.50
ATOM	613	SD	MET	1535	1.722	2.764	11.628	1.00	22.97
ATOM	614	CE	MET	1535	1.681	4.534	11.727	1.00	23.90
ATOM	615	C	MET	1535	-0.725	0.540	7.572	1.00	30.33
ATOM	616	O	MET	1535	-0.636	-0.694	7.706	1.00	33.31
ATOM	617	N	LYS	1536	-1.823	1.135	7.104	1.00	28.91
ATOM	619	CA	LYS	1536	-3.011	0.364	6.732	1.00	28.07
ATOM	620	CB	LYS	1536	-4.176	1.289	6.413	1.00	25.52
ATOM	621	CG	LYS	1536	-4.689	2.080	7.579	1.00	21.46
ATOM	622	CD	LYS	1536	-5.810	2.979	7.127	1.00	19.89

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ATOM	623	CE	LYS	1536	-6.414	3.717	8.288	1.00	23.50
ATOM	624	NZ	LYS	1536	-7.469	4.668	7.850	1.00	23.53
ATOM	628	C	LYS	1536	-2.765	-0.542	5.530	1.00	29.09
ATOM	629	O	LYS	1536	-3.127	-1.708	5.550	1.00	34.02
ATOM	630	N	MET	1537	-2.141	-0.009	4.488	1.00	29.03
ATOM	632	CA	MET	1537	-1.869	-0.792	3.288	1.00	30.13
ATOM	633	CB	MET	1537	-1.315	0.111	2.177	1.00	31.96
ATOM	634	CG	MET	1537	-2.304	1.114	1.589	1.00	35.15
ATOM	635	SD	MET	1537	-3.757	0.380	0.787	1.00	41.18
ATOM	636	CE	MET	1537	-3.026	-0.360	-0.666	1.00	43.05
ATOM	637	C	MET	1537	-0.905	-1.946	3.531	1.00	30.22
ATOM	638	O	MET	1537	-1.118	-3.051	3.045	1.00	30.88
ATOM	639	N	ILE	1538	0.164	-1.686	4.275	1.00	30.91
ATOM	641	CA	ILE	1538	1.192	-2.701	4.536	1.00	30.29
ATOM	642	CB	ILE	1538	2.429	-2.082	5.221	1.00	28.64
ATOM	643	CG2	ILE	1538	3.493	-3.142	5.453	1.00	29.84
ATOM	644	CG1	ILE	1538	3.025	-1.030	4.287	1.00	32.82
ATOM	645	CD1	ILE	1538	4.358	-0.446	4.763	1.00	38.38
ATOM	646	C	ILE	1538	0.759	-4.000	5.237	1.00	29.07
ATOM	647	O	ILE	1538	1.229	-5.078	4.876	1.00	28.30
ATOM	648	N	GLY	1539	-0.178	-3.925	6.174	1.00	27.61
ATOM	650	CA	GLY	1539	-0.592	-5.147	6.849	1.00	26.22
ATOM	651	C	GLY	1539	0.273	-5.484	8.055	1.00	25.67
ATOM	652	O	GLY	1539	1.345	-4.906	8.241	1.00	28.05
ATOM	653	N	LYS	1540	-0.150	-6.483	8.819	1.00	23.80
ATOM	655	CA	LYS	1540	0.532	-6.876	10.046	1.00	21.77
ATOM	656	CB	LYS	1540	-0.491	-7.436	11.045	1.00	20.04
ATOM	657	CG	LYS	1540	-1.505	-6.435	11.480	1.00	24.45
ATOM	658	CD	LYS	1540	-2.472	-6.997	12.488	1.00	32.57
ATOM	659	CE	LYS	1540	-3.516	-5.946	12.882	1.00	35.05
ATOM	660	NZ	LYS	1540	-2.959	-4.850	13.733	1.00	39.81
ATOM	664	C	LYS	1540	1.669	-7.862	9.958	1.00	20.19
ATOM	665	O	LYS	1540	1.671	-8.738	9.099	1.00	21.80
ATOM	666	N	HIS	1541	2.626	-7.722	10.876	1.00	19.98
ATOM	668	CA	HIS	1541	3.770	-8.626	11.000	1.00	22.43
ATOM	669	CB	HIS	1541	4.854	-8.374	9.965	1.00	22.34
ATOM	670	CG	HIS	1541	5.892	-9.455	9.923	1.00	20.68
ATOM	671	CD2	HIS	1541	5.906	-10.654	9.295	1.00	20.60
ATOM	672	ND1	HIS	1541	7.074	-9.382	10.633	1.00	23.67
ATOM	674	CE1	HIS	1541	7.771	-10.490	10.444	1.00	23.35
ATOM	675	NE2	HIS	1541	7.087	-11.278	9.634	1.00	22.04
ATOM	677	C	HIS	1541	4.385	-8.477	12.376	1.00	27.21
ATOM	678	O	HIS	1541	4.538	-7.367	12.885	1.00	31.33
ATOM	679	N	LYS	1542	4.726	-9.619	12.958	1.00	29.25
ATOM	681	CA	LYS	1542	5.319	-9.698	14.285	1.00	30.39
ATOM	682	CB	LYS	1542	5.660	-11.151	14.610	1.00	33.76
ATOM	683	CG	LYS	1542	6.232	-11.370	15.994	1.00	42.16
ATOM	684	CD	LYS	1542	6.400	-12.833	16.230	1.00	49.69
ATOM	685	CE	LYS	1542	7.040	-13.499	14.988	1.00	57.71
ATOM	686	NZ	LYS	1542	7.499	-14.904	15.237	1.00	62.05
ATOM	690	C	LYS	1542	6.515	-8.808	14.462	1.00	27.21
ATOM	691	O	LYS	1542	6.690	-8.232	15.522	1.00	29.68

ATOM	692	N	ASN	1543	7.293	-8.619	13.410	1.00	23.81
ATOM	694	CA	ASN	1543	8.472	-7.787	13.537	1.00	24.70
ATOM	695	CB	ASN	1543	9.697	-8.550	13.031	1.00	24.68
ATOM	696	CG	ASN	1543	9.914	-9.855	13.793	1.00	24.82
ATOM	697	OD1	ASN	1543	9.734	-10.942	13.239	1.00	27.33
ATOM	698	ND2	ASN	1543	10.255	-9.758	15.078	1.00	16.75
ATOM	701	C	ASN	1543	8.444	-6.326	13.032	1.00	24.93
ATOM	702	O	ASN	1543	9.469	-5.781	12.623	1.00	26.76
ATOM	703	N	ILE	1544	7.276	-5.692	13.088	1.00	24.21
ATOM	705	CA	ILE	1544	7.121	-4.281	12.710	1.00	21.87
ATOM	706	CB	ILE	1544	6.626	-4.095	11.240	1.00	23.23
ATOM	707	CG2	ILE	1544	7.549	-4.837	10.267	1.00	23.87
ATOM	708	CG1	ILE	1544	5.182	-4.580	11.063	1.00	22.57
ATOM	709	CD1	ILE	1544	4.639	-4.342	9.659	1.00	17.59
ATOM	710	C	ILE	1544	6.122	-3.656	13.696	1.00	21.64
ATOM	711	O	ILE	1544	5.399	-4.377	14.397	1.00	21.00
ATOM	712	N	ILE	1545	6.167	-2.340	13.856	1.00	21.59
ATOM	714	CA	ILE	1545	5.214	-1.687	14.746	1.00	24.05
ATOM	715	CB	ILE	1545	5.641	-0.242	15.138	1.00	23.68
ATOM	716	CG2	ILE	1545	4.473	0.500	15.831	1.00	21.90
ATOM	717	CG1	ILE	1545	6.880	-0.284	16.050	1.00	21.94
ATOM	718	CD1	ILE	1545	6.643	-0.808	17.446	1.00	9.18
ATOM	719	C	ILE	1545	3.914	-1.641	13.955	1.00	25.08
ATOM	720	O	ILE	1545	3.842	-1.001	12.897	1.00	26.68
ATOM	721	N	ASN	1546	2.909	-2.358	14.455	1.00	25.88
ATOM	723	CA	ASN	1546	1.602	-2.424	13.800	1.00	24.61
ATOM	724	CB	ASN	1546	0.944	-3.793	14.005	1.00	23.18
ATOM	725	CG	ASN	1546	1.759	-4.923	13.434	1.00	21.54
ATOM	726	OD1	ASN	1546	1.884	-5.059	12.214	1.00	21.52
ATOM	727	ND2	ASN	1546	2.319	-5.748	14.313	1.00	18.83
ATOM	730	C	ASN	1546	0.646	-1.368	14.292	1.00	23.02
ATOM	731	O	ASN	1546	0.739	-0.911	15.429	1.00	25.66
ATOM	732	N	LEU	1547	-0.285	-1.014	13.422	1.00	24.45
ATOM	734	CA	LEU	1547	-1.336	-0.041	13.692	1.00	24.27
ATOM	735	CB	LEU	1547	-1.819	0.553	12.360	1.00	18.04
ATOM	736	CG	LEU	1547	-3.012	1.515	12.343	1.00	19.96
ATOM	737	CD1	LEU	1547	-2.630	2.928	12.842	1.00	10.60
ATOM	738	CD2	LEU	1547	-3.555	1.570	10.924	1.00	16.44
ATOM	739	C	LEU	1547	-2.469	-0.826	14.384	1.00	26.95
ATOM	740	O	LEU	1547	-2.835	-1.934	13.956	1.00	27.38
ATOM	741	N	LEU	1548	-2.998	-0.260	15.460	1.00	26.61
ATOM	743	CA	LEU	1548	-4.063	-0.902	16.222	1.00	26.25
ATOM	744	CB	LEU	1548	-3.717	-0.951	17.721	1.00	22.48
ATOM	745	CG	LEU	1548	-2.370	-1.553	18.117	1.00	20.24
ATOM	746	CD1	LEU	1548	-2.282	-1.656	19.616	1.00	19.27
ATOM	747	CD2	LEU	1548	-2.175	-2.929	17.492	1.00	19.23
ATOM	748	C	LEU	1548	-5.401	-0.198	16.017	1.00	26.75
ATOM	749	O	LEU	1548	-6.447	-0.837	16.036	1.00	25.56
ATOM	750	N	GLY	1549	-5.367	1.115	15.823	1.00	25.78
ATOM	752	CA	GLY	1549	-6.607	1.843	15.616	1.00	25.80
ATOM	753	C	GLY	1549	-6.319	3.324	15.490	1.00	27.76
ATOM	754	O	GLY	1549	-5.148	3.716	15.405	1.00	28.05

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ATOM	755	N	ALA	1550	-7.369	4.143	15.530	1.00	27.34
ATOM	757	CA	ALA	1550	-7.212	5.582	15.414	1.00	25.85
ATOM	758	CB	ALA	1550	-6.925	5.947	13.978	1.00	23.09
ATOM	759	C	ALA	1550	-8.430	6.353	15.897	1.00	26.58
ATOM	760	O	ALA	1550	-9.562	5.866	15.797	1.00	28.26
ATOM	761	N	CYS	1551	-8.182	7.551	16.429	1.00	26.30
ATOM	763	CA	CYS	1551	-9.227	8.471	16.899	1.00	28.29
ATOM	764	CB	CYS	1551	-8.966	8.952	18.342	1.00	27.12
ATOM	765	SG	CYS	1551	-9.101	7.681	19.630	1.00	27.09
ATOM	766	C	CYS	1551	-9.092	9.646	15.934	1.00	28.57
ATOM	767	O	CYS	1551	-8.156	10.436	16.044	1.00	26.80
ATOM	768	N	THR	1552	-9.966	9.699	14.933	1.00	29.27
ATOM	770	CA	THR	1552	-9.889	10.736	13.921	1.00	29.30
ATOM	771	CB	THR	1552	-9.779	10.110	12.495	1.00	27.19
ATOM	772	OG1	THR	1552	-10.978	9.393	12.191	1.00	26.68
ATOM	774	CG2	THR	1552	-8.629	9.133	12.414	1.00	27.00
ATOM	775	C	THR	1552	-11.045	11.716	13.905	1.00	29.86
ATOM	776	O	THR	1552	-10.918	12.838	13.403	1.00	30.69
ATOM	777	N	GLN	1553	-12.201	11.268	14.369	1.00	31.21
ATOM	779	CA	GLN	1553	-13.374	12.124	14.329	1.00	34.31
ATOM	780	CB	GLN	1553	-14.641	11.279	14.147	1.00	33.00
ATOM	781	CG	GLN	1553	-14.714	10.530	12.820	1.00	34.68
ATOM	782	CD	GLN	1553	-14.584	11.453	11.617	1.00	39.26
ATOM	783	OE1	GLN	1553	-15.300	12.449	11.506	1.00	43.55
ATOM	784	NE2	GLN	1553	-13.668	11.129	10.718	1.00	37.56
ATOM	787	C	GLN	1553	-13.502	13.040	15.526	1.00	36.86
ATOM	788	O	GLN	1553	-13.030	12.714	16.613	1.00	34.88
ATOM	789	N	ASP	1554	-14.122	14.195	15.290	1.00	40.73
ATOM	791	CA	ASP	1554	-14.369	15.202	16.313	1.00	42.49
ATOM	792	CB	ASP	1554	-15.693	14.913	17.028	1.00	46.26
ATOM	793	CG	ASP	1554	-16.907	15.174	16.153	1.00	51.14
ATOM	794	OD1	ASP	1554	-17.686	16.097	16.488	1.00	57.62
ATOM	795	OD2	ASP	1554	-17.092	14.463	15.146	1.00	55.72
ATOM	796	C	ASP	1554	-13.249	15.299	17.336	1.00	42.31
ATOM	797	O	ASP	1554	-13.443	14.955	18.501	1.00	43.61
ATOM	798	N	GLY	1555	-12.077	15.753	16.902	1.00	41.03
ATOM	800	CA	GLY	1555	-10.960	15.864	17.823	1.00	37.98
ATOM	801	C	GLY	1555	-9.605	15.674	17.167	1.00	38.30
ATOM	802	O	GLY	1555	-9.533	15.478	15.953	1.00	37.28
ATOM	803	N	PRO	1556	-8.511	15.693	17.961	1.00	37.62
ATOM	804	CD	PRO	1556	-8.575	15.755	19.429	1.00	37.23
ATOM	805	CA	PRO	1556	-7.123	15.533	17.500	1.00	33.79
ATOM	806	CB	PRO	1556	-6.296	15.748	18.773	1.00	33.33
ATOM	807	CG	PRO	1556	-7.254	16.353	19.770	1.00	36.99
ATOM	808	C	PRO	1556	-6.891	14.134	16.990	1.00	33.57
ATOM	809	O	PRO	1556	-7.378	13.175	17.568	1.00	32.10
ATOM	810	N	LEU	1557	-6.168	14.031	15.884	1.00	33.23
ATOM	812	CA	LEU	1557	-5.859	12.745	15.300	1.00	34.20
ATOM	813	CB	LEU	1557	-5.173	12.950	13.944	1.00	32.88
ATOM	814	CG	LEU	1557	-4.674	11.716	13.183	1.00	29.78
ATOM	815	CD1	LEU	1557	-5.810	10.730	12.943	1.00	29.22
ATOM	816	CD2	LEU	1557	-4.085	12.161	11.880	1.00	28.17

ATOM	817	C	LEU	1557	-4.950	11.927	16.225	1.00	36.29
ATOM	818	O	LEU	1557	-3.847	12.365	16.580	1.00	37.50
ATOM	819	N	TYR	1558	-5.427	10.765	16.658	1.00	35.35
ATOM	821	CA	TYR	1558	-4.619	9.890	17.495	1.00	33.09
ATOM	822	CB	TYR	1558	-5.323	9.516	18.805	1.00	34.16
ATOM	823	CG	TYR	1558	-5.363	10.629	19.806	1.00	34.40
ATOM	824	CD1	TYR	1558	-6.364	10.688	20.771	1.00	33.23
ATOM	825	CE1	TYR	1558	-6.438	11.747	21.663	1.00	34.52
ATOM	826	CD2	TYR	1558	-4.426	11.655	19.757	1.00	37.30
ATOM	827	CE2	TYR	1558	-4.488	12.715	20.640	1.00	38.44
ATOM	828	CZ	TYR	1558	-5.494	12.762	21.587	1.00	36.17
ATOM	829	OH	TYR	1558	-5.561	13.848	22.431	1.00	34.28
ATOM	831	C	TYR	1558	-4.379	8.627	16.700	1.00	31.12
ATOM	832	O	TYR	1558	-5.329	7.980	16.255	1.00	29.83
ATOM	833	N	VAL	1559	-3.109	8.321	16.468	1.00	29.60
ATOM	835	CA	VAL	1559	-2.727	7.115	15.753	1.00	27.08
ATOM	836	CB	VAL	1559	-1.647	7.420	14.704	1.00	24.96
ATOM	837	CG1	VAL	1559	-1.281	6.149	13.926	1.00	24.36
ATOM	838	CG2	VAL	1559	-2.147	8.525	13.765	1.00	19.21
ATOM	839	C	VAL	1559	-2.238	6.102	16.794	1.00	25.65
ATOM	840	O	VAL	1559	-1.169	6.257	17.389	1.00	24.97
ATOM	841	N	ILE	1560	-3.067	5.095	17.046	1.00	25.91
ATOM	843	CA	ILE	1560	-2.777	4.062	18.042	1.00	26.94
ATOM	844	CB	ILE	1560	-4.081	3.530	18.637	1.00	24.89
ATOM	845	CG2	ILE	1560	-3.785	2.744	19.900	1.00	17.89
ATOM	846	CG1	ILE	1560	-5.028	4.707	18.907	1.00	22.84
ATOM	847	CD1	ILE	1560	-6.450	4.304	19.163	1.00	22.51
ATOM	848	C	ILE	1560	-1.955	2.896	17.467	1.00	30.61
ATOM	849	O	ILE	1560	-2.445	2.111	16.636	1.00	31.41
ATOM	850	N	VAL	1561	-0.698	2.811	17.890	1.00	30.26
ATOM	852	CA	VAL	1561	0.222	1.779	17.429	1.00	29.39
ATOM	853	CB	VAL	1561	1.466	2.437	16.730	1.00	30.18
ATOM	854	CG1	VAL	1561	1.030	3.188	15.475	1.00	20.60
ATOM	855	CG2	VAL	1561	2.148	3.415	17.675	1.00	32.91
ATOM	856	C	VAL	1561	0.662	0.870	18.588	1.00	27.40
ATOM	857	O	VAL	1561	0.323	1.128	19.742	1.00	29.33
ATOM	858	N	GLU	1562	1.381	-0.209	18.279	1.00	24.75
ATOM	860	CA	GLU	1562	1.852	-1.142	19.308	1.00	22.64
ATOM	861	CB	GLU	1562	2.426	-2.410	18.676	1.00	17.97
ATOM	862	CG	GLU	1562	1.365	-3.282	18.029	1.00	24.33
ATOM	863	CD	GLU	1562	1.909	-4.552	17.383	1.00	26.80
ATOM	864	OE1	GLU	1562	1.247	-5.592	17.507	1.00	33.32
ATOM	865	OE2	GLU	1562	2.974	-4.538	16.722	1.00	25.62
ATOM	866	C	GLU	1562	2.885	-0.534	20.259	1.00	25.09
ATOM	867	O	GLU	1562	3.638	0.355	19.899	1.00	23.82
ATOM	868	N	TYR	1563	2.897	-1.023	21.491	1.00	28.01
ATOM	870	CA	TYR	1563	3.805	-0.539	22.512	1.00	26.93
ATOM	871	CB	TYR	1563	3.045	-0.428	23.829	1.00	27.19
ATOM	872	CG	TYR	1563	3.868	0.008	25.009	1.00	27.72
ATOM	873	CD1	TYR	1563	4.581	1.196	24.976	1.00	30.61
ATOM	874	CE1	TYR	1563	5.303	1.620	26.069	1.00	33.05
ATOM	875	CD2	TYR	1563	3.908	-0.753	26.176	1.00	25.77

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ATOM	876	CE2	TYR	1563	4.626	-0.344	27.267	1.00	26.81
ATOM	877	CZ	TYR	1563	5.329	0.845	27.210	1.00	32.81
ATOM	878	OH	TYR	1563	6.091	1.271	28.276	1.00	40.16
ATOM	880	C	TYR	1563	4.989	-1.487	22.675	1.00	28.73
ATOM	881	O	TYR	1563	4.815	-2.704	22.735	1.00	27.05
ATOM	882	N	ALA	1564	6.189	-0.908	22.743	1.00	29.89
ATOM	884	CA	ALA	1564	7.453	-1.634	22.916	1.00	28.50
ATOM	885	CB	ALA	1564	8.392	-1.349	21.721	1.00	27.54
ATOM	886	C	ALA	1564	8.036	-1.092	24.229	1.00	27.05
ATOM	887	O	ALA	1564	8.790	-0.129	24.249	1.00	31.20
ATOM	888	N	SER	1565	7.650	-1.706	25.333	1.00	27.11
ATOM	890	CA	SER	1565	8.062	-1.251	26.652	1.00	28.91
ATOM	891	CB	SER	1565	7.501	-2.152	27.729	1.00	27.33
ATOM	892	OG	SER	1565	8.108	-3.419	27.650	1.00	26.58
ATOM	894	C	SER	1565	9.530	-1.085	26.915	1.00	30.19
ATOM	895	O	SER	1565	9.897	-0.330	27.810	1.00	33.44
ATOM	896	N	LYS	1566	10.368	-1.801	26.178	1.00	30.99
ATOM	898	CA	LYS	1566	11.798	-1.708	26.410	1.00	30.50
ATOM	899	CB	LYS	1566	12.452	-3.082	26.335	1.00	30.38
ATOM	900	CG	LYS	1566	12.037	-3.943	27.507	1.00	27.83
ATOM	901	CD	LYS	1566	12.605	-5.339	27.457	1.00	32.36
ATOM	902	CE	LYS	1566	12.345	-6.024	28.784	1.00	30.57
ATOM	903	NZ	LYS	1566	12.651	-7.460	28.722	1.00	34.82
ATOM	907	C	LYS	1566	12.526	-0.678	25.573	1.00	30.39
ATOM	908	O	LYS	1566	13.755	-0.567	25.640	1.00	32.53
ATOM	909	N	GLY	1567	11.753	0.127	24.851	1.00	29.45
ATOM	911	CA	GLY	1567	12.319	1.184	24.035	1.00	29.17
ATOM	912	C	GLY	1567	13.079	0.742	22.806	1.00	28.14
ATOM	913	O	GLY	1567	12.875	-0.364	22.324	1.00	27.70
ATOM	914	N	ASN	1568	13.975	1.601	22.320	1.00	29.48
ATOM	916	CA	ASN	1568	14.754	1.308	21.121	1.00	30.00
ATOM	917	CB	ASN	1568	15.271	2.591	20.464	1.00	28.53
ATOM	918	CG	ASN	1568	16.342	3.285	21.281	1.00	30.13
ATOM	919	OD1	ASN	1568	17.305	2.670	21.730	1.00	31.50
ATOM	920	ND2	ASN	1568	16.212	4.591	21.420	1.00	30.91
ATOM	923	C	ASN	1568	15.892	0.333	21.352	1.00	28.83
ATOM	924	O	ASN	1568	16.371	0.201	22.472	1.00	29.87
ATOM	925	N	LEU	1569	16.346	-0.300	20.274	1.00	27.43
ATOM	927	CA	LEU	1569	17.417	-1.291	20.323	1.00	29.95
ATOM	928	CB	LEU	1569	17.511	-2.022	18.972	1.00	28.96
ATOM	929	CG	LEU	1569	18.508	-3.173	18.797	1.00	30.82
ATOM	930	CD1	LEU	1569	18.431	-4.211	19.939	1.00	28.31
ATOM	931	CD2	LEU	1569	18.244	-3.819	17.461	1.00	25.70
ATOM	932	C	LEU	1569	18.805	-0.779	20.754	1.00	29.74
ATOM	933	O	LEU	1569	19.530	-1.484	21.447	1.00	28.35
ATOM	934	N	ARG	1570	19.179	0.427	20.341	1.00	31.42
ATOM	936	CA	ARG	1570	20.485	0.985	20.703	1.00	32.81
ATOM	937	CB	ARG	1570	20.639	2.395	20.115	1.00	31.01
ATOM	938	CG	ARG	1570	21.922	3.091	20.543	1.00	35.33
ATOM	939	CD	ARG	1570	21.918	4.581	20.212	1.00	38.30
ATOM	940	NE	ARG	1570	20.700	5.272	20.649	1.00	47.77
ATOM	942	CZ	ARG	1570	20.393	5.595	21.912	1.00	53.56

ATOM	943	NH1	ARG	1570	21.212	5.304	22.931	1.00	51.30
ATOM	946	NH2	ARG	1570	19.245	6.223	22.161	1.00	51.34
ATOM	949	C	ARG	1570	20.620	1.034	22.230	1.00	35.61
ATOM	950	O	ARG	1570	21.548	0.455	22.814	1.00	34.40
ATOM	951	N	GLU	1571	19.677	1.724	22.863	1.00	36.79
ATOM	953	CA	GLU	1571	19.637	1.855	24.311	1.00	37.35
ATOM	954	CB	GLU	1571	18.403	2.662	24.725	1.00	41.36
ATOM	955	CG	GLU	1571	18.407	4.118	24.267	1.00	49.97
ATOM	956	CD	GLU	1571	17.048	4.823	24.459	1.00	59.14
ATOM	957	OE1	GLU	1571	15.991	4.133	24.595	1.00	59.21
ATOM	958	OE2	GLU	1571	17.043	6.081	24.446	1.00	59.41
ATOM	959	C	GLU	1571	19.593	0.459	24.948	1.00	37.09
ATOM	960	O	GLU	1571	20.327	0.172	25.892	1.00	37.70
ATOM	961	N	TYR	1572	18.750	-0.405	24.400	1.00	35.08
ATOM	963	CA	TYR	1572	18.591	-1.766	24.878	1.00	32.72
ATOM	964	CB	TYR	1572	17.571	-2.499	23.995	1.00	31.62
ATOM	965	CG	TYR	1572	17.376	-3.973	24.309	1.00	25.69
ATOM	966	CD1	TYR	1572	16.392	-4.378	25.187	1.00	27.87
ATOM	967	CE1	TYR	1572	16.180	-5.711	25.458	1.00	28.57
ATOM	968	CD2	TYR	1572	18.151	-4.941	23.703	1.00	22.18
ATOM	969	CE2	TYR	1572	17.948	-6.284	23.969	1.00	25.06
ATOM	970	CZ	TYR	1572	16.954	-6.659	24.852	1.00	25.65
ATOM	971	OH	TYR	1572	16.732	-7.985	25.143	1.00	25.29
ATOM	973	C	TYR	1572	19.904	-2.525	24.871	1.00	34.57
ATOM	974	O	TYR	1572	20.186	-3.309	25.796	1.00	35.05
ATOM	975	N	LEU	1573	20.692	-2.338	23.812	1.00	33.34
ATOM	977	CA	LEU	1573	21.970	-3.033	23.712	1.00	33.00
ATOM	978	CB	LEU	1573	22.487	-3.018	22.273	1.00	28.86
ATOM	979	CG	LEU	1573	21.833	-3.888	21.198	1.00	23.37
ATOM	980	CD1	LEU	1573	22.339	-3.448	19.840	1.00	16.57
ATOM	981	CD2	LEU	1573	22.129	-5.354	21.426	1.00	20.31
ATOM	982	C	LEU	1573	22.997	-2.417	24.655	1.00	36.57
ATOM	983	O	LEU	1573	23.752	-3.134	25.311	1.00	39.00
ATOM	984	N	GLN	1574	23.003	-1.090	24.735	1.00	37.26
ATOM	986	CA	GLN	1574	23.942	-0.399	25.608	1.00	37.50
ATOM	987	CB	GLN	1574	23.844	1.110	25.394	1.00	36.96
ATOM	988	CG	GLN	1574	24.526	1.582	24.113	1.00	39.10
ATOM	989	CD	GLN	1574	24.289	3.054	23.801	1.00	40.63
ATOM	990	OE1	GLN	1574	23.697	3.796	24.595	1.00	38.68
ATOM	991	NE2	GLN	1574	24.736	3.480	22.625	1.00	38.62
ATOM	994	C	GLN	1574	23.687	-0.759	27.073	1.00	38.27
ATOM	995	O	GLN	1574	24.600	-1.144	27.801	1.00	39.43
ATOM	996	N	ALA	1575	22.422	-0.731	27.469	1.00	38.80
ATOM	998	CA	ALA	1575	22.021	-1.044	28.831	1.00	39.51
ATOM	999	CB	ALA	1575	20.551	-0.714	29.024	1.00	36.89
ATOM	1000	C	ALA	1575	22.304	-2.484	29.275	1.00	40.89
ATOM	1001	O	ALA	1575	22.006	-2.842	30.417	1.00	44.53
ATOM	1002	N	ARG	1576	22.857	-3.317	28.395	1.00	39.11
ATOM	1004	CA	ARG	1576	23.148	-4.703	28.768	1.00	38.24
ATOM	1005	CB	ARG	1576	22.234	-5.669	28.019	1.00	38.42
ATOM	1006	CG	ARG	1576	20.794	-5.518	28.472	1.00	39.73
ATOM	1007	CD	ARG	1576	19.838	-6.352	27.687	1.00	37.87

ATOM	1008	NE	ARG	1576	18.489	-6.260	28.235	1.00	41.03
ATOM	1010	CZ	ARG	1576	17.830	-5.123	28.436	1.00	43.27
ATOM	1011	NH1	ARG	1576	18.399	-3.961	28.143	1.00	42.64
ATOM	1014	NH2	ARG	1576	16.573	-5.152	28.877	1.00	46.13
ATOM	1017	C	ARG	1576	24.604	-5.076	28.612	1.00	39.77
ATOM	1018	O	ARG	1576	24.978	-6.256	28.623	1.00	40.25
ATOM	1019	N	ARG	1577	25.428	-4.042	28.501	1.00	40.39
ATOM	1021	CA	ARG	1577	26.866	-4.194	28.388	1.00	40.42
ATOM	1022	CB	ARG	1577	27.485	-2.871	27.952	1.00	37.67
ATOM	1023	CG	ARG	1577	27.247	-2.477	26.526	1.00	36.22
ATOM	1024	CD	ARG	1577	27.857	-1.113	26.287	1.00	35.55
ATOM	1025	NE	ARG	1577	27.971	-0.797	24.866	1.00	38.72
ATOM	1027	CZ	ARG	1577	28.395	0.369	24.384	1.00	37.57
ATOM	1028	NH1	ARG	1577	28.754	1.352	25.205	1.00	37.49
ATOM	1031	NH2	ARG	1577	28.449	0.562	23.074	1.00	39.58
ATOM	1034	C	ARG	1577	27.449	-4.548	29.760	1.00	42.45
ATOM	1035	O	ARG	1577	26.878	-4.180	30.801	1.00	42.57
ATOM	1036	N	PRO	1578	28.564	-5.296	29.797	1.00	43.36
ATOM	1037	CD	PRO	1578	29.270	-5.985	28.692	1.00	42.43
ATOM	1038	CA	PRO	1578	29.159	-5.648	31.082	1.00	43.08
ATOM	1039	CB	PRO	1578	30.225	-6.676	30.709	1.00	40.33
ATOM	1040	CG	PRO	1578	30.600	-6.300	29.331	1.00	40.71
ATOM	1041	C	PRO	1578	29.768	-4.373	31.666	1.00	42.44
ATOM	1042	O	PRO	1578	30.261	-3.525	30.922	1.00	41.24
ATOM	1043	N	PRO	1579	29.705	-4.205	32.993	1.00	44.57
ATOM	1044	CD	PRO	1579	29.169	-5.143	33.994	1.00	46.68
ATOM	1045	CA	PRO	1579	30.251	-3.017	33.654	1.00	44.89
ATOM	1046	CB	PRO	1579	30.088	-3.356	35.134	1.00	45.31
ATOM	1047	CG	PRO	1579	28.865	-4.224	35.142	1.00	44.45
ATOM	1048	C	PRO	1579	31.711	-2.767	33.289	1.00	45.17
ATOM	1049	O	PRO	1579	32.620	-3.257	33.953	1.00	47.72
ATOM	1050	N	ALA	1592	19.075	-5.384	32.475	1.00	49.23
ATOM	1052	CA	ALA	1592	20.500	-5.078	32.354	1.00	50.33
ATOM	1053	CB	ALA	1592	20.954	-4.184	33.503	1.00	51.83
ATOM	1054	C	ALA	1592	21.412	-6.308	32.251	1.00	50.65
ATOM	1055	O	ALA	1592	22.621	-6.166	32.044	1.00	51.55
ATOM	1056	N	ALA	1593	20.849	-7.505	32.409	1.00	49.06
ATOM	1058	CA	ALA	1593	21.638	-8.735	32.294	1.00	48.07
ATOM	1059	CB	ALA	1593	20.773	-9.953	32.579	1.00	47.87
ATOM	1060	C	ALA	1593	22.258	-8.840	30.891	1.00	47.59
ATOM	1061	O	ALA	1593	21.664	-8.426	29.894	1.00	49.09
ATOM	1062	N	GLN	1594	23.465	-9.388	30.830	1.00	47.30
ATOM	1064	CA	GLN	1594	24.186	-9.553	29.569	1.00	45.32
ATOM	1065	CB	GLN	1594	25.576	-10.118	29.837	1.00	44.82
ATOM	1066	CG	GLN	1594	26.523	-9.166	30.542	1.00	49.34
ATOM	1067	CD	GLN	1594	27.751	-9.877	31.111	1.00	52.40
ATOM	1068	OE1	GLN	1594	28.264	-10.847	30.537	1.00	51.16
ATOM	1069	NE2	GLN	1594	28.209	-9.408	32.265	1.00	54.00
ATOM	1072	C	GLN	1594	23.474	-10.432	28.539	1.00	45.00
ATOM	1073	O	GLN	1594	22.780	-11.393	28.876	1.00	45.28
ATOM	1074	N	LEU	1595	23.684	-10.104	27.273	1.00	45.08
ATOM	1076	CA	LEU	1595	23.084	-10.828	26.169	1.00	44.65

ATOM	1077	CB	LEU	1595	22.758	-9.864	25.023	1.00	43.08
ATOM	1078	CG	LEU	1595	21.619	-8.877	25.295	1.00	43.22
ATOM	1079	CD1	LEU	1595	21.855	-7.563	24.564	1.00	41.25
ATOM	1080	CD2	LEU	1595	20.276	-9.510	24.918	1.00	41.96
ATOM	1081	C	LEU	1595	24.044	-11.885	25.685	1.00	44.58
ATOM	1082	O	LEU	1595	25.252	-11.661	25.632	1.00	44.62
ATOM	1083	N	SER	1596	23.511	-13.058	25.376	1.00	45.71
ATOM	1085	CA	SER	1596	24.325	-14.151	24.868	1.00	45.30
ATOM	1086	CB	SER	1596	23.633	-15.495	25.124	1.00	46.19
ATOM	1087	OG	SER	1596	22.401	-15.605	24.432	1.00	44.03
ATOM	1089	C	SER	1596	24.557	-13.968	23.366	1.00	45.09
ATOM	1090	O	SER	1596	23.891	-13.156	22.707	1.00	45.03
ATOM	1091	N	SER	1597	25.475	-14.756	22.823	1.00	44.55
ATOM	1093	CA	SER	1597	25.782	-14.690	21.407	1.00	45.00
ATOM	1094	CB	SER	1597	26.921	-15.643	21.065	1.00	45.60
ATOM	1095	OG	SER	1597	27.976	-15.516	22.007	1.00	54.80
ATOM	1097	C	SER	1597	24.526	-15.076	20.633	1.00	43.92
ATOM	1098	O	SER	1597	24.233	-14.498	19.577	1.00	45.51
ATOM	1099	N	LYS	1598	23.767	-16.025	21.178	1.00	39.36
ATOM	1101	CA	LYS	1598	22.551	-16.454	20.519	1.00	36.56
ATOM	1102	CB	LYS	1598	21.978	-17.715	21.147	1.00	34.93
ATOM	1103	CG	LYS	1598	21.374	-18.643	20.101	1.00	37.52
ATOM	1104	CD	LYS	1598	20.450	-19.665	20.706	1.00	34.85
ATOM	1105	CE	LYS	1598	20.054	-20.709	19.702	1.00	30.95
ATOM	1106	NZ	LYS	1598	21.219	-21.551	19.334	1.00	30.59
ATOM	1110	C	LYS	1598	21.521	-15.336	20.552	1.00	36.21
ATOM	1111	O	LYS	1598	20.840	-15.099	19.548	1.00	36.39
ATOM	1112	N	ASP	1599	21.447	-14.624	21.681	1.00	33.57
ATOM	1114	CA	ASP	1599	20.520	-13.508	21.841	1.00	31.94
ATOM	1115	CB	ASP	1599	20.635	-12.898	23.238	1.00	33.82
ATOM	1116	CG	ASP	1599	20.143	-13.838	24.339	1.00	38.08
ATOM	1117	OD1	ASP	1599	20.659	-13.717	25.475	1.00	37.52
ATOM	1118	OD2	ASP	1599	19.256	-14.691	24.072	1.00	36.17
ATOM	1119	C	ASP	1599	20.777	-12.430	20.802	1.00	30.89
ATOM	1120	O	ASP	1599	19.846	-11.945	20.153	1.00	30.88
ATOM	1121	N	LEU	1600	22.046	-12.070	20.636	1.00	31.39
ATOM	1123	CA	LEU	1600	22.439	-11.050	19.666	1.00	31.55
ATOM	1124	CB	LEU	1600	23.921	-10.695	19.845	1.00	30.47
ATOM	1125	CG	LEU	1600	24.341	-10.072	21.190	1.00	29.24
ATOM	1126	CD1	LEU	1600	25.857	-9.923	21.226	1.00	29.75
ATOM	1127	CD2	LEU	1600	23.666	-8.731	21.404	1.00	24.50
ATOM	1128	C	LEU	1600	22.136	-11.478	18.212	1.00	31.39
ATOM	1129	O	LEU	1600	21.620	-10.686	17.418	1.00	31.23
ATOM	1130	N	VAL	1601	22.439	-12.729	17.863	1.00	30.00
ATOM	1132	CA	VAL	1601	22.161	-13.231	16.518	1.00	27.94
ATOM	1133	CB	VAL	1601	22.827	-14.600	16.261	1.00	27.68
ATOM	1134	CG1	VAL	1601	22.467	-15.108	14.885	1.00	24.69
ATOM	1135	CG2	VAL	1601	24.326	-14.474	16.362	1.00	25.87
ATOM	1136	C	VAL	1601	20.642	-13.340	16.310	1.00	28.98
ATOM	1137	O	VAL	1601	20.152	-13.151	15.191	1.00	28.55
ATOM	1138	N	SER	1602	19.904	-13.635	17.382	1.00	27.64
ATOM	1140	CA	SER	1602	18.450	-13.726	17.318	1.00	27.07

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ATOM	1141	CB	SER	1602	17.899	-14.362	18.584	1.00	29.97	
ATOM	1142	OG	SER	1602	16.488	-14.202	18.673	1.00	38.86	
ATOM	1144	C	SER	1602	17.864	-12.327	17.093	1.00	27.45	
ATOM	1145	O	SER	1602	16.826	-12.181	16.438	1.00	29.38	
ATOM	1146	N	CYS	1603	18.504	-11.306	17.663	1.00	25.31	
ATOM	1148	CA	CYS	1603	18.087	-9.909	17.461	1.00	24.49	
ATOM	1149	CB	CYS	1603	19.074	-8.965	18.143	1.00	21.15	
ATOM	1150	SG	CYS	1603	18.716	-7.213	18.030	0.50	11.83	PRT1
ATOM	1151	C	CYS	1603	18.155	-9.628	15.961	1.00	26.92	
ATOM	1152	O	CYS	1603	17.175	-9.238	15.329	1.00	30.04	
ATOM	1153	N	ALA	1604	19.340	-9.833	15.398	1.00	28.35	
ATOM	1155	CA	ALA	1604	19.573	-9.611	13.979	1.00	28.00	
ATOM	1156	CB	ALA	1604	20.970	-10.098	13.588	1.00	25.49	
ATOM	1157	C	ALA	1604	18.517	-10.295	13.132	1.00	26.69	
ATOM	1158	O	ALA	1604	17.892	-9.646	12.310	1.00	31.40	
ATOM	1159	N	TYR	1605	18.270	-11.577	13.399	1.00	26.33	
ATOM	1161	CA	TYR	1605	17.286	-12.384	12.666	1.00	24.79	
ATOM	1162	CB	TYR	1605	17.209	-13.771	13.300	1.00	23.42	
ATOM	1163	CG	TYR	1605	16.132	-14.663	12.742	1.00	29.93	
ATOM	1164	CD1	TYR	1605	16.281	-15.298	11.510	1.00	30.00	
ATOM	1165	CE1	TYR	1605	15.270	-16.097	10.989	1.00	32.29	
ATOM	1166	CD2	TYR	1605	14.949	-14.859	13.441	1.00	32.69	
ATOM	1167	CE2	TYR	1605	13.935	-15.650	12.934	1.00	33.02	
ATOM	1168	CZ	TYR	1605	14.091	-16.266	11.713	1.00	34.40	
ATOM	1169	OH	TYR	1605	13.037	-17.023	11.225	1.00	34.18	
ATOM	1171	C	TYR	1605	15.885	-11.750	12.572	1.00	26.08	
ATOM	1172	O	TYR	1605	15.327	-11.587	11.475	1.00	25.43	
ATOM	1173	N	GLN	1606	15.337	-11.366	13.717	1.00	25.38	
ATOM	1175	CA	GLN	1606	14.018	-10.737	13.776	1.00	25.47	
ATOM	1176	CB	GLN	1606	13.662	-10.424	15.227	1.00	24.21	
ATOM	1177	CG	GLN	1606	13.642	-11.636	16.127	1.00	24.37	
ATOM	1178	CD	GLN	1606	13.237	-11.279	17.540	1.00	27.16	
ATOM	1179	OE1	GLN	1606	12.227	-10.603	17.758	1.00	29.64	
ATOM	1180	NE2	GLN	1606	14.033	-11.705	18.507	1.00	30.69	
ATOM	1183	C	GLN	1606	13.953	-9.449	12.949	1.00	26.89	
ATOM	1184	O	GLN	1606	12.936	-9.136	12.319	1.00	26.40	
ATOM	1185	N	VAL	1607	15.030	-8.674	13.000	1.00	27.79	
ATOM	1187	CA	VAL	1607	15.120	-7.430	12.255	1.00	26.35	
ATOM	1188	CB	VAL	1607	16.408	-6.667	12.625	1.00	24.87	
ATOM	1189	CG1	VAL	1607	16.556	-5.433	11.752	1.00	25.90	
ATOM	1190	CG2	VAL	1607	16.382	-6.282	14.094	1.00	17.95	
ATOM	1191	C	VAL	1607	15.121	-7.743	10.757	1.00	27.69	
ATOM	1192	O	VAL	1607	14.406	-7.093	9.979	1.00	30.85	
ATOM	1193	N	ALA	1608	15.902	-8.749	10.355	1.00	24.59	
ATOM	1195	CA	ALA	1608	15.965	-9.135	8.950	1.00	23.22	
ATOM	1196	CB	ALA	1608	16.971	-10.227	8.750	1.00	17.65	
ATOM	1197	C	ALA	1608	14.579	-9.589	8.492	1.00	24.58	
ATOM	1198	O	ALA	1608	14.201	-9.372	7.337	1.00	26.22	
ATOM	1199	N	ARG	1609	13.819	-10.191	9.409	1.00	25.65	
ATOM	1201	CA	ARG	1609	12.453	-10.648	9.124	1.00	24.86	
ATOM	1202	CB	ARG	1609	11.998	-11.660	10.160	1.00	28.15	
ATOM	1203	CG	ARG	1609	12.451	-13.050	9.863	1.00	30.10	

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ATOM	1204	CD	ARG	1609	11.683	-13.980	10.723	1.00	32.49
ATOM	1205	NE	ARG	1609	10.942	-14.941	9.927	1.00	34.58
ATOM	1207	CZ	ARG	1609	10.058	-15.792	10.437	1.00	35.69
ATOM	1208	NH1	ARG	1609	9.800	-15.790	11.740	1.00	32.47
ATOM	1211	NH2	ARG	1609	9.468	-16.678	9.645	1.00	36.67
ATOM	1214	C	ARG	1609	11.421	-9.518	9.008	1.00	22.96
ATOM	1215	O	ARG	1609	10.522	-9.582	8.155	1.00	23.65
ATOM	1216	N	GLY	1610	11.501	-8.522	9.888	1.00	20.88
ATOM	1218	CA	GLY	1610	10.591	-7.398	9.789	1.00	21.47
ATOM	1219	C	GLY	1610	10.822	-6.741	8.432	1.00	23.55
ATOM	1220	O	GLY	1610	9.872	-6.452	7.688	1.00	23.53
ATOM	1221	N	MET	1611	12.097	-6.558	8.088	1.00	24.37
ATOM	1223	CA	MET	1611	12.488	-5.955	6.809	1.00	25.10
ATOM	1224	CB	MET	1611	13.991	-5.686	6.801	1.00	25.47
ATOM	1225	CG	MET	1611	14.391	-4.478	7.652	1.00	27.09
ATOM	1226	SD	MET	1611	13.362	-3.000	7.330	1.00	22.57
ATOM	1227	CE	MET	1611	13.665	-2.715	5.612	1.00	21.91
ATOM	1228	C	MET	1611	12.090	-6.791	5.590	1.00	26.57
ATOM	1229	O	MET	1611	11.700	-6.251	4.553	1.00	24.98
ATOM	1230	N	GLU	1612	12.213	-8.108	5.710	1.00	27.89
ATOM	1232	CA	GLU	1612	11.836	-9.002	4.632	1.00	26.91
ATOM	1233	CB	GLU	1612	12.120	-10.446	5.024	1.00	26.70
ATOM	1234	CG	GLU	1612	11.602	-11.443	4.026	1.00	29.25
ATOM	1235	CD	GLU	1612	11.796	-12.872	4.477	1.00	31.24
ATOM	1236	OE1	GLU	1612	11.658	-13.143	5.692	1.00	33.39
ATOM	1237	OE2	GLU	1612	12.085	-13.733	3.617	1.00	31.91
ATOM	1238	C	GLU	1612	10.354	-8.812	4.305	1.00	27.55
ATOM	1239	O	GLU	1612	9.974	-8.697	3.130	1.00	30.04
ATOM	1240	N	TYR	1613	9.518	-8.752	5.337	1.00	25.13
ATOM	1242	CA	TYR	1613	8.092	-8.545	5.133	1.00	21.91
ATOM	1243	CB	TYR	1613	7.341	-8.625	6.462	1.00	21.00
ATOM	1244	CG	TYR	1613	5.867	-8.318	6.335	1.00	17.47
ATOM	1245	CD1	TYR	1613	4.969	-9.307	5.968	1.00	18.34
ATOM	1246	CE1	TYR	1613	3.610	-9.049	5.872	1.00	18.83
ATOM	1247	CD2	TYR	1613	5.373	-7.041	6.600	1.00	14.48
ATOM	1248	CE2	TYR	1613	4.017	-6.761	6.502	1.00	19.67
ATOM	1249	CZ	TYR	1613	3.137	-7.776	6.135	1.00	22.67
ATOM	1250	OH	TYR	1613	1.779	-7.542	6.009	1.00	21.91
ATOM	1252	C	TYR	1613	7.870	-7.170	4.504	1.00	22.06
ATOM	1253	O	TYR	1613	7.125	-7.034	3.540	1.00	22.01
ATOM	1254	N	LEU	1614	8.541	-6.154	5.045	1.00	22.04
ATOM	1256	CA	LEU	1614	8.400	-4.794	4.536	1.00	20.56
ATOM	1257	CB	LEU	1614	9.219	-3.830	5.392	1.00	18.43
ATOM	1258	CG	LEU	1614	8.548	-3.413	6.707	1.00	15.96
ATOM	1259	CD1	LEU	1614	9.509	-2.571	7.518	1.00	15.70
ATOM	1260	CD2	LEU	1614	7.255	-2.647	6.436	1.00	11.06
ATOM	1261	C	LEU	1614	8.793	-4.671	3.066	1.00	22.69
ATOM	1262	O	LEU	1614	8.156	-3.939	2.294	1.00	24.91
ATOM	1263	N	ALA	1615	9.840	-5.397	2.684	1.00	24.55
ATOM	1265	CA	ALA	1615	10.333	-5.408	1.317	1.00	21.18
ATOM	1266	CB	ALA	1615	11.685	-6.088	1.254	1.00	18.35
ATOM	1267	C	ALA	1615	9.334	-6.107	0.404	1.00	21.97

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ATOM	1268	O	ALA	1615	9.089	-5.642	-0.705	1.00	23.80
ATOM	1269	N	SER	1616	8.704	-7.173	0.893	1.00	22.49
ATOM	1271	CA	SER	1616	7.722	-7.919	0.097	1.00	21.81
ATOM	1272	CB	SER	1616	7.305	-9.179	0.831	1.00	19.78
ATOM	1273	OG	SER	1616	6.382	-8.862	1.851	1.00	23.88
ATOM	1275	C	SER	1616	6.475	-7.071	-0.149	1.00	23.60
ATOM	1276	O	SER	1616	5.733	-7.277	-1.117	1.00	21.74
ATOM	1277	N	LYS	1617	6.217	-6.169	0.789	1.00	25.84
ATOM	1279	CA	LYS	1617	5.078	-5.280	0.705	1.00	23.96
ATOM	1280	CB	LYS	1617	4.555	-4.951	2.099	1.00	20.74
ATOM	1281	CG	LYS	1617	3.843	-6.124	2.750	1.00	23.40
ATOM	1282	CD	LYS	1617	2.509	-6.395	2.081	1.00	28.70
ATOM	1283	CE	LYS	1617	1.714	-7.442	2.809	1.00	31.16
ATOM	1284	NZ	LYS	1617	2.339	-8.767	2.616	1.00	41.91
ATOM	1288	C	LYS	1617	5.409	-4.019	-0.061	1.00	24.25
ATOM	1289	O	LYS	1617	4.640	-3.053	-0.022	1.00	25.22
ATOM	1290	N	LYS	1618	6.557	-4.028	-0.748	1.00	24.20
ATOM	1292	CA	LYS	1618	7.014	-2.904	-1.582	1.00	25.15
ATOM	1293	CB	LYS	1618	5.906	-2.507	-2.571	1.00	27.00
ATOM	1294	CG	LYS	1618	5.735	-3.411	-3.790	1.00	29.09
ATOM	1295	CD	LYS	1618	5.506	-4.864	-3.432	1.00	31.82
ATOM	1296	CE	LYS	1618	5.533	-5.752	-4.663	1.00	30.21
ATOM	1297	NZ	LYS	1618	4.231	-5.707	-5.369	1.00	26.34
ATOM	1301	C	LYS	1618	7.466	-1.658	-0.816	1.00	23.50
ATOM	1302	O	LYS	1618	7.537	-0.576	-1.385	1.00	22.10
ATOM	1303	N	CYS	1619	7.827	-1.821	0.449	1.00	23.72
ATOM	1305	CA	CYS	1619	8.213	-0.693	1.276	1.00	20.89
ATOM	1306	CB	CYS	1619	7.535	-0.814	2.647	1.00	18.41
ATOM	1307	SG	CYS	1619	8.019	0.405	3.894	1.00	26.34
ATOM	1308	C	CYS	1619	9.717	-0.529	1.451	1.00	22.94
ATOM	1309	O	CYS	1619	10.419	-1.487	1.790	1.00	23.20
ATOM	1310	N	ILE	1620	10.197	0.690	1.211	1.00	21.17
ATOM	1312	CA	ILE	1620	11.610	1.039	1.388	1.00	22.35
ATOM	1313	CB	ILE	1620	12.151	1.823	0.172	1.00	17.30
ATOM	1314	CG2	ILE	1620	13.607	2.215	0.393	1.00	8.27
ATOM	1315	CG1	ILE	1620	11.966	0.997	-1.111	1.00	18.27
ATOM	1316	CD1	ILE	1620	12.127	1.803	-2.401	1.00	17.57
ATOM	1317	C	ILE	1620	11.631	1.926	2.652	1.00	25.20
ATOM	1318	O	ILE	1620	10.912	2.932	2.715	1.00	29.69
ATOM	1319	N	HIS	1621	12.398	1.526	3.665	1.00	22.66
ATOM	1321	CA	HIS	1621	12.463	2.254	4.931	1.00	22.78
ATOM	1322	CB	HIS	1621	13.214	1.425	5.980	1.00	22.65
ATOM	1323	CG	HIS	1621	13.024	1.897	7.398	1.00	22.07
ATOM	1324	CD2	HIS	1621	12.485	1.280	8.475	1.00	20.50
ATOM	1325	ND1	HIS	1621	13.449	3.134	7.842	1.00	23.11
ATOM	1327	CE1	HIS	1621	13.182	3.253	9.131	1.00	23.92
ATOM	1328	NE2	HIS	1621	12.596	2.144	9.543	1.00	24.44
ATOM	1330	C	HIS	1621	13.110	3.616	4.831	1.00	24.07
ATOM	1331	O	HIS	1621	12.561	4.597	5.306	1.00	24.37
ATOM	1332	N	ARG	1622	14.327	3.639	4.291	1.00	26.42
ATOM	1334	CA	ARG	1622	15.129	4.853	4.130	1.00	24.59
ATOM	1335	CB	ARG	1622	14.289	6.018	3.581	1.00	17.58

ATOM	1336	CG	ARG	1622	13.810	5.767	2.163	1.00	13.88
ATOM	1337	CD	ARG	1622	12.925	6.860	1.634	0.50	4.97
ATOM	1338	NE	ARG	1622	12.574	6.590	0.243	0.50	6.49
ATOM	1340	CZ	ARG	1622	11.537	5.852	-0.145	0.50	3.84
ATOM	1341	NH1	ARG	1622	10.719	5.308	0.753	0.50	2.25
ATOM	1344	NH2	ARG	1622	11.356	5.611	-1.433	0.50	2.48
ATOM	1347	C	ARG	1622	15.918	5.257	5.388	1.00	24.72
ATOM	1348	O	ARG	1622	16.767	6.138	5.337	1.00	26.90
ATOM	1349	N	ASP	1623	15.685	4.585	6.505	1.00	25.61
ATOM	1351	CA	ASP	1623	16.437	4.927	7.703	1.00	28.41
ATOM	1352	CB	ASP	1623	15.922	6.213	8.349	1.00	30.38
ATOM	1353	CG	ASP	1623	16.891	6.772	9.373	1.00	33.47
ATOM	1354	OD1	ASP	1623	16.428	7.338	10.382	1.00	43.35
ATOM	1355	OD2	ASP	1623	18.121	6.645	9.167	1.00	31.88
ATOM	1356	C	ASP	1623	16.498	3.797	8.713	1.00	28.86
ATOM	1357	O	ASP	1623	16.148	3.959	9.887	1.00	28.31
ATOM	1358	N	LEU	1624	16.956	2.642	8.246	1.00	27.81
ATOM	1360	CA	LEU	1624	17.087	1.480	9.107	1.00	27.28
ATOM	1361	CB	LEU	1624	17.149	0.220	8.242	1.00	27.53
ATOM	1362	CG	LEU	1624	17.118	-1.150	8.916	1.00	27.69
ATOM	1363	CD1	LEU	1624	15.850	-1.348	9.756	1.00	23.77
ATOM	1364	CD2	LEU	1624	17.228	-2.175	7.805	1.00	29.15
ATOM	1365	C	LEU	1624	18.340	1.628	10.002	1.00	26.27
ATOM	1366	O	LEU	1624	19.464	1.773	9.514	1.00	25.89
ATOM	1367	N	ALA	1625	18.116	1.598	11.313	1.00	23.29
ATOM	1369	CA	ALA	1625	19.164	1.750	12.314	1.00	19.68
ATOM	1370	CB	ALA	1625	19.520	3.233	12.473	1.00	18.85
ATOM	1371	C	ALA	1625	18.575	1.214	13.613	1.00	20.79
ATOM	1372	O	ALA	1625	17.352	1.077	13.716	1.00	20.75
ATOM	1373	N	ALA	1626	19.429	0.942	14.605	1.00	22.03
ATOM	1375	CA	ALA	1626	18.969	0.408	15.900	1.00	23.43
ATOM	1376	CB	ALA	1626	20.139	-0.048	16.764	1.00	22.46
ATOM	1377	C	ALA	1626	18.111	1.397	16.664	1.00	25.86
ATOM	1378	O	ALA	1626	17.333	1.006	17.523	1.00	29.51
ATOM	1379	N	ARG	1627	18.303	2.685	16.407	1.00	26.92
ATOM	1381	CA	ARG	1627	17.503	3.722	17.048	1.00	27.30
ATOM	1382	CB	ARG	1627	18.017	5.107	16.627	1.00	28.29
ATOM	1383	CG	ARG	1627	18.086	5.287	15.104	1.00	36.26
ATOM	1384	CD	ARG	1627	18.255	6.756	14.688	1.00	41.19
ATOM	1385	NE	ARG	1627	18.548	6.928	13.261	1.00	39.94
ATOM	1387	CZ	ARG	1627	19.779	6.904	12.749	1.00	42.33
ATOM	1388	NH1	ARG	1627	20.826	6.721	13.539	1.00	44.75
ATOM	1391	NH2	ARG	1627	19.976	7.059	11.450	1.00	41.50
ATOM	1394	C	ARG	1627	16.029	3.567	16.591	1.00	27.42
ATOM	1395	O	ARG	1627	15.092	3.897	17.333	1.00	26.53
ATOM	1396	N	ASN	1628	15.850	3.039	15.375	1.00	26.82
ATOM	1398	CA	ASN	1628	14.534	2.849	14.758	1.00	24.08
ATOM	1399	CB	ASN	1628	14.569	3.308	13.301	1.00	26.30
ATOM	1400	CG	ASN	1628	14.709	4.823	13.167	1.00	25.19
ATOM	1401	OD1	ASN	1628	14.018	5.567	13.844	1.00	28.59
ATOM	1402	ND2	ASN	1628	15.599	5.277	12.297	1.00	22.32
ATOM	1405	C	ASN	1628	13.945	1.440	14.862	1.00	24.35

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ATOM	1406	O	ASN	1628	13.026	1.084	14.105	1.00	24.66
ATOM	1407	N	VAL	1629	14.473	0.637	15.785	1.00	22.35
ATOM	1409	CA	VAL	1629	13.988	-0.718	16.055	1.00	20.65
ATOM	1410	CB	VAL	1629	15.077	-1.813	15.822	1.00	18.07
ATOM	1411	CG1	VAL	1629	14.612	-3.142	16.398	1.00	11.84
ATOM	1412	CG2	VAL	1629	15.378	-1.977	14.346	1.00	12.65
ATOM	1413	C	VAL	1629	13.625	-0.670	17.536	1.00	24.27
ATOM	1414	O	VAL	1629	14.427	-0.237	18.361	1.00	25.94
ATOM	1415	N	LEU	1630	12.393	-1.031	17.866	1.00	24.99
ATOM	1417	CA	LEU	1630	11.936	-1.010	19.247	1.00	25.50
ATOM	1418	CB	LEU	1630	10.609	-0.252	19.339	1.00	22.79
ATOM	1419	CG	LEU	1630	10.634	1.179	18.789	1.00	17.86
ATOM	1420	CD1	LEU	1630	9.240	1.680	18.654	1.00	18.49
ATOM	1421	CD2	LEU	1630	11.409	2.100	19.668	1.00	17.63
ATOM	1422	C	LEU	1630	11.833	-2.434	19.829	1.00	28.29
ATOM	1423	O	LEU	1630	11.666	-3.412	19.092	1.00	28.56
ATOM	1424	N	VAL	1631	11.933	-2.542	21.150	1.00	29.46
ATOM	1426	CA	VAL	1631	11.883	-3.831	21.833	1.00	29.40
ATOM	1427	CB	VAL	1631	13.222	-4.105	22.553	1.00	27.48
ATOM	1428	CG1	VAL	1631	13.210	-5.477	23.233	1.00	24.53
ATOM	1429	CG2	VAL	1631	14.376	-3.976	21.576	1.00	22.55
ATOM	1430	C	VAL	1631	10.730	-3.918	22.853	1.00	31.94
ATOM	1431	O	VAL	1631	10.630	-3.102	23.787	1.00	33.13
ATOM	1432	N	THR	1632	9.866	-4.911	22.659	1.00	32.21
ATOM	1434	CA	THR	1632	8.728	-5.149	23.540	1.00	31.77
ATOM	1435	CB	THR	1632	7.674	-6.061	22.874	1.00	32.38
ATOM	1436	OG1	THR	1632	8.169	-7.406	22.792	1.00	32.38
ATOM	1438	CG2	THR	1632	7.330	-5.554	21.480	1.00	28.05
ATOM	1439	C	THR	1632	9.157	-5.810	24.842	1.00	30.39
ATOM	1440	O	THR	1632	10.256	-6.320	24.947	1.00	30.28
ATOM	1441	N	GLU	1633	8.260	-5.823	25.822	1.00	32.43
ATOM	1443	CA	GLU	1633	8.513	-6.424	27.122	1.00	32.84
ATOM	1444	CB	GLU	1633	7.259	-6.310	27.991	1.00	35.28
ATOM	1445	CG	GLU	1633	7.386	-6.881	29.399	1.00	46.57
ATOM	1446	CD	GLU	1633	8.463	-6.192	30.260	1.00	54.03
ATOM	1447	OE1	GLU	1633	8.519	-4.939	30.297	1.00	58.68
ATOM	1448	OE2	GLU	1633	9.249	-6.916	30.918	1.00	56.84
ATOM	1449	C	GLU	1633	8.914	-7.889	26.986	1.00	35.14
ATOM	1450	O	GLU	1633	9.632	-8.435	27.826	1.00	33.92
ATOM	1451	N	ASP	1634	8.456	-8.526	25.910	1.00	38.25
ATOM	1453	CA	ASP	1634	8.768	-9.941	25.677	1.00	39.22
ATOM	1454	CB	ASP	1634	7.588	-10.639	24.990	1.00	44.88
ATOM	1455	CG	ASP	1634	6.258	-10.420	25.725	1.00	54.17
ATOM	1456	OD1	ASP	1634	6.064	-11.042	26.799	1.00	56.33
ATOM	1457	OD2	ASP	1634	5.412	-9.622	25.236	1.00	54.47
ATOM	1458	C	ASP	1634	10.035	-10.109	24.849	1.00	37.53
ATOM	1459	O	ASP	1634	10.395	-11.225	24.495	1.00	36.33
ATOM	1460	N	ASN	1635	10.730	-8.998	24.589	1.00	39.12
ATOM	1462	CA	ASN	1635	11.974	-8.948	23.792	1.00	37.21
ATOM	1463	CB	ASN	1635	13.042	-9.891	24.361	1.00	37.83
ATOM	1464	CG	ASN	1635	13.576	-9.426	25.677	1.00	38.65
ATOM	1465	OD1	ASN	1635	13.795	-8.236	25.880	1.00	43.82

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ATOM	1466	ND2	ASN	1635	13.768	-10.353	26.596	1.00	39.49
ATOM	1469	C	ASN	1635	11.807	-9.193	22.287	1.00	35.03
ATOM	1470	O	ASN	1635	12.649	-9.834	21.648	1.00	32.37
ATOM	1471	N	VAL	1636	10.705	-8.700	21.736	1.00	33.30
ATOM	1473	CA	VAL	1636	10.418	-8.846	20.320	1.00	30.50
ATOM	1474	CB	VAL	1636	8.895	-9.014	20.075	1.00	31.54
ATOM	1475	CG1	VAL	1636	8.600	-9.178	18.584	1.00	29.16
ATOM	1476	CG2	VAL	1636	8.384	-10.214	20.838	1.00	34.29
ATOM	1477	C	VAL	1636	10.908	-7.577	19.629	1.00	29.28
ATOM	1478	O	VAL	1636	10.553	-6.463	20.037	1.00	27.08
ATOM	1479	N	MET	1637	11.760	-7.755	18.623	1.00	27.82
ATOM	1481	CA	MET	1637	12.318	-6.634	17.874	1.00	27.09
ATOM	1482	CB	MET	1637	13.578	-7.070	17.127	1.00	27.47
ATOM	1483	CG	MET	1637	14.648	-7.697	18.010	1.00	28.35
ATOM	1484	SD	MET	1637	15.243	-6.594	19.297	1.00	30.41
ATOM	1485	CE	MET	1637	15.104	-7.640	20.728	1.00	26.00
ATOM	1486	C	MET	1637	11.272	-6.200	16.868	1.00	26.01
ATOM	1487	O	MET	1637	10.751	-7.034	16.131	1.00	26.05
ATOM	1488	N	LYS	1638	10.983	-4.900	16.823	1.00	25.44
ATOM	1490	CA	LYS	1638	9.984	-4.349	15.906	1.00	22.01
ATOM	1491	CB	LYS	1638	8.693	-4.028	16.658	1.00	19.65
ATOM	1492	CG	LYS	1638	7.887	-5.254	17.034	1.00	21.22
ATOM	1493	CD	LYS	1638	6.666	-4.904	17.869	1.00	21.73
ATOM	1494	CE	LYS	1638	5.776	-6.133	18.076	1.00	19.32
ATOM	1495	NZ	LYS	1638	4.970	-6.522	16.869	1.00	23.14
ATOM	1499	C	LYS	1638	10.477	-3.106	15.191	1.00	21.85
ATOM	1500	O	LYS	1638	10.896	-2.147	15.808	1.00	24.35
ATOM	1501	N	ILE	1639	10.371	-3.110	13.878	1.00	24.47
ATOM	1503	CA	ILE	1639	10.803	-1.983	13.073	1.00	24.90
ATOM	1504	CB	ILE	1639	11.090	-2.443	11.625	1.00	22.12
ATOM	1505	CG2	ILE	1639	11.413	-1.275	10.720	1.00	17.41
ATOM	1506	CG1	ILE	1639	12.256	-3.423	11.664	1.00	18.67
ATOM	1507	CD1	ILE	1639	12.309	-4.308	10.492	1.00	26.15
ATOM	1508	C	ILE	1639	9.772	-0.856	13.117	1.00	28.52
ATOM	1509	O	ILE	1639	8.557	-1.094	12.964	1.00	27.86
ATOM	1510	N	ALA	1640	10.267	0.363	13.358	1.00	30.06
ATOM	1512	CA	ALA	1640	9.444	1.564	13.445	1.00	29.37
ATOM	1513	CB	ALA	1640	9.627	2.211	14.812	1.00	28.25
ATOM	1514	C	ALA	1640	9.782	2.566	12.344	1.00	29.68
ATOM	1515	O	ALA	1640	10.808	2.453	11.660	1.00	30.81
ATOM	1516	N	ASP	1641	8.892	3.536	12.154	1.00	30.35
ATOM	1518	CA	ASP	1641	9.067	4.608	11.154	1.00	30.40
ATOM	1519	CB	ASP	1641	10.309	5.454	11.454	1.00	32.89
ATOM	1520	CG	ASP	1641	10.018	6.678	12.321	1.00	34.68
ATOM	1521	OD1	ASP	1641	10.952	7.497	12.469	1.00	35.84
ATOM	1522	OD2	ASP	1641	8.897	6.824	12.856	1.00	38.22
ATOM	1523	C	ASP	1641	9.102	4.162	9.705	1.00	28.91
ATOM	1524	O	ASP	1641	9.484	4.941	8.826	1.00	29.26
ATOM	1525	N	PHE	1642	8.650	2.941	9.440	1.00	27.21
ATOM	1527	CA	PHE	1642	8.648	2.435	8.072	1.00	25.07
ATOM	1528	CB	PHE	1642	8.432	0.909	8.043	1.00	19.64
ATOM	1529	CG	PHE	1642	7.135	0.451	8.639	1.00	16.47

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ATOM	1530	CD1	PHE	1642	5.974	0.400	7.878	1.00	21.72
ATOM	1531	CD2	PHE	1642	7.080	0.018	9.945	1.00	17.01
ATOM	1532	CE1	PHE	1642	4.781	-0.082	8.422	1.00	20.97
ATOM	1533	CE2	PHE	1642	5.892	-0.463	10.496	1.00	18.72
ATOM	1534	CZ	PHE	1642	4.743	-0.515	9.739	1.00	20.32
ATOM	1535	C	PHE	1642	7.667	3.174	7.157	1.00	25.57
ATOM	1536	O	PHE	1642	7.910	3.292	5.971	1.00	28.40
ATOM	1537	N	GLY	1643	6.585	3.718	7.707	1.00	25.69
ATOM	1539	CA	GLY	1643	5.631	4.427	6.866	1.00	24.81
ATOM	1540	C	GLY	1643	5.786	5.935	6.893	1.00	24.84
ATOM	1541	O	GLY	1643	4.922	6.684	6.436	1.00	19.20
ATOM	1542	N	LEU	1644	6.930	6.387	7.376	1.00	29.50
ATOM	1544	CA	LEU	1644	7.189	7.808	7.491	1.00	34.24
ATOM	1545	CB	LEU	1644	8.498	8.037	8.242	1.00	33.10
ATOM	1546	CG	LEU	1644	8.473	9.371	8.962	1.00	36.00
ATOM	1547	CD1	LEU	1644	7.520	9.212	10.127	1.00	41.52
ATOM	1548	CD2	LEU	1644	9.854	9.773	9.442	1.00	35.23
ATOM	1549	C	LEU	1644	7.213	8.578	6.179	1.00	37.54
ATOM	1550	O	LEU	1644	7.759	8.123	5.176	1.00	37.48
ATOM	1551	N	ALA	1645	6.577	9.744	6.203	1.00	41.66
ATOM	1553	CA	ALA	1645	6.524	10.652	5.067	1.00	43.66
ATOM	1554	CB	ALA	1645	5.309	11.563	5.202	1.00	38.13
ATOM	1555	C	ALA	1645	7.819	11.475	5.141	1.00	44.67
ATOM	1556	O	ALA	1645	8.105	12.082	6.176	1.00	47.17
ATOM	1557	N	ALA	1646	8.622	11.462	4.082	1.00	45.69
ATOM	1559	CA	ALA	1646	9.871	12.222	4.094	1.00	48.62
ATOM	1560	CB	ALA	1646	10.971	11.405	4.778	1.00	49.50
ATOM	1561	C	ALA	1646	10.338	12.661	2.712	1.00	50.98
ATOM	1562	O	ALA	1646	10.319	11.880	1.759	1.00	52.84
ATOM	1563	N	ASP	1647	10.755	13.919	2.598	1.00	53.09
ATOM	1565	CA	ASP	1647	11.253	14.419	1.322	1.00	55.06
ATOM	1566	CB	ASP	1647	10.868	15.887	1.092	1.00	56.05
ATOM	1567	CG	ASP	1647	11.084	16.342	-0.352	1.00	59.31
ATOM	1568	OD1	ASP	1647	12.070	15.928	-1.003	1.00	59.51
ATOM	1569	OD2	ASP	1647	10.265	17.150	-0.837	1.00	63.48
ATOM	1570	C	ASP	1647	12.770	14.264	1.332	1.00	55.26
ATOM	1571	O	ASP	1647	13.487	15.075	1.926	1.00	53.18
ATOM	1572	N	ILE	1648	13.235	13.198	0.684	1.00	56.66
ATOM	1574	CA	ILE	1648	14.652	12.877	0.595	1.00	57.79
ATOM	1575	CB	ILE	1648	14.890	11.624	-0.271	1.00	53.86
ATOM	1576	CG2	ILE	1648	14.133	10.443	0.326	1.00	52.14
ATOM	1577	CG1	ILE	1648	14.454	11.886	-1.718	1.00	48.24
ATOM	1578	CD1	ILE	1648	15.198	11.083	-2.751	1.00	43.97
ATOM	1579	C	ILE	1648	15.439	14.044	0.014	1.00	62.32
ATOM	1580	O	ILE	1648	16.591	14.271	0.380	1.00	64.72
ATOM	1581	N	HIS	1649	14.805	14.791	-0.884	1.00	65.72
ATOM	1583	CA	HIS	1649	15.450	15.941	-1.500	1.00	69.00
ATOM	1584	CB	HIS	1649	14.793	16.285	-2.844	1.00	70.35
ATOM	1585	CG	HIS	1649	15.123	15.332	-3.944	1.00	73.90
ATOM	1586	CD2	HIS	1649	16.257	14.628	-4.208	1.00	75.13
ATOM	1587	ND1	HIS	1649	14.239	15.006	-4.946	1.00	75.30
ATOM	1589	CE1	HIS	1649	14.798	14.148	-5.779	1.00	76.83

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ATOM	1590	NE2	HIS	1649	16.025	13.905	-5.348	1.00	76.74
ATOM	1592	C	HIS	1649	15.419	17.150	-0.576	1.00	70.22
ATOM	1593	O	HIS	1649	15.517	18.284	-1.041	1.00	72.83
ATOM	1594	N	HIS	1650	15.218	16.912	0.718	1.00	71.28
ATOM	1596	CA	HIS	1650	15.199	17.987	1.710	1.00	72.52
ATOM	1597	CB	HIS	1650	13.776	18.488	1.956	1.00	75.67
ATOM	1598	CG	HIS	1650	13.272	19.401	0.882	1.00	82.16
ATOM	1599	CD2	HIS	1650	13.451	20.734	0.691	1.00	86.17
ATOM	1600	ND1	HIS	1650	12.529	18.955	-0.185	1.00	86.37
ATOM	1602	CE1	HIS	1650	12.262	19.972	-0.993	1.00	89.04
ATOM	1603	NE2	HIS	1650	12.814	21.058	-0.481	1.00	89.37
ATOM	1605	C	HIS	1650	15.856	17.593	3.029	1.00	71.11
ATOM	1606	O	HIS	1650	15.783	18.334	4.010	1.00	69.56
ATOM	1607	N	ILE	1651	16.543	16.451	3.033	1.00	70.84
ATOM	1609	CA	ILE	1651	17.221	15.939	4.222	1.00	70.50
ATOM	1610	CB	ILE	1651	17.622	14.462	4.031	1.00	71.73
ATOM	1611	CG2	ILE	1651	18.499	13.978	5.194	1.00	71.65
ATOM	1612	CG1	ILE	1651	16.359	13.604	3.890	1.00	73.10
ATOM	1613	CD1	ILE	1651	16.643	12.143	3.593	1.00	75.18
ATOM	1614	C	ILE	1651	18.472	16.734	4.569	1.00	69.85
ATOM	1615	O	ILE	1651	19.375	16.882	3.745	1.00	70.30
ATOM	1616	N	ASP	1652	18.543	17.222	5.802	1.00	68.99
ATOM	1618	CA	ASP	1652	19.707	17.987	6.240	1.00	68.06
ATOM	1619	CB	ASP	1652	19.344	18.923	7.398	1.00	70.53
ATOM	1620	CG	ASP	1652	20.512	19.790	7.843	1.00	72.86
ATOM	1621	OD1	ASP	1652	21.306	20.248	6.985	1.00	73.36
ATOM	1622	OD2	ASP	1652	20.646	20.034	9.060	1.00	76.01
ATOM	1623	C	ASP	1652	20.802	17.023	6.673	1.00	66.08
ATOM	1624	O	ASP	1652	20.746	16.457	7.762	1.00	64.92
ATOM	1625	N	TYR	1653	21.802	16.856	5.814	1.00	64.14
ATOM	1627	CA	TYR	1653	22.926	15.968	6.089	1.00	63.02
ATOM	1628	CB	TYR	1653	23.852	15.906	4.875	1.00	61.29
ATOM	1629	CG	TYR	1653	23.362	14.971	3.795	1.00	62.37
ATOM	1630	CD1	TYR	1653	24.153	14.679	2.684	1.00	61.11
ATOM	1631	CE1	TYR	1653	23.725	13.773	1.717	1.00	62.89
ATOM	1632	CD2	TYR	1653	22.121	14.335	3.910	1.00	64.11
ATOM	1633	CE2	TYR	1653	21.685	13.429	2.953	1.00	66.09
ATOM	1634	CZ	TYR	1653	22.487	13.148	1.859	1.00	65.03
ATOM	1635	OH	TYR	1653	22.044	12.239	0.921	1.00	65.78
ATOM	1637	C	TYR	1653	23.733	16.313	7.345	1.00	63.49
ATOM	1638	O	TYR	1653	24.403	15.453	7.912	1.00	63.39
ATOM	1639	N	TYR	1654	23.644	17.564	7.789	1.00	64.37
ATOM	1641	CA	TYR	1654	24.379	18.013	8.963	1.00	63.95
ATOM	1642	CB	TYR	1654	24.947	19.417	8.741	1.00	60.86
ATOM	1643	CG	TYR	1654	26.038	19.467	7.691	1.00	57.70
ATOM	1644	CD1	TYR	1654	25.736	19.698	6.353	1.00	58.03
ATOM	1645	CE1	TYR	1654	26.734	19.708	5.383	1.00	60.65
ATOM	1646	CD2	TYR	1654	27.364	19.252	8.035	1.00	56.79
ATOM	1647	CE2	TYR	1654	28.366	19.261	7.079	1.00	58.85
ATOM	1648	CZ	TYR	1654	28.047	19.488	5.754	1.00	60.88
ATOM	1649	OH	TYR	1654	29.048	19.485	4.806	1.00	64.23
ATOM	1651	C	TYR	1654	23.560	17.980	10.239	1.00	65.89

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ATOM	1652	O	TYR	1654	24.074	18.283	11.316	1.00	67.56
ATOM	1653	N	LYS	1655	22.297	17.586	10.135	1.00	67.36
ATOM	1655	CA	LYS	1655	21.443	17.527	11.315	1.00	69.11
ATOM	1656	CB	LYS	1655	19.972	17.611	10.915	1.00	69.86
ATOM	1657	CG	LYS	1655	19.019	17.651	12.090	1.00	71.45
ATOM	1658	CD	LYS	1655	17.607	17.867	11.603	1.00	75.40
ATOM	1659	CE	LYS	1655	16.595	17.393	12.627	1.00	78.22
ATOM	1660	NZ	LYS	1655	15.204	17.553	12.110	1.00	80.61
ATOM	1664	C	LYS	1655	21.714	16.242	12.093	1.00	69.65
ATOM	1665	O	LYS	1655	21.872	15.169	11.497	1.00	70.67
ATOM	1666	N	LYS	1656	21.766	16.358	13.419	1.00	68.19
ATOM	1668	CA	LYS	1656	22.035	15.212	14.275	1.00	68.00
ATOM	1669	CB	LYS	1656	22.983	15.618	15.403	1.00	65.53
ATOM	1670	CG	LYS	1656	24.395	15.895	14.946	1.00	62.71
ATOM	1671	CD	LYS	1656	25.280	16.221	16.138	1.00	64.38
ATOM	1672	CE	LYS	1656	26.764	16.031	15.832	1.00	63.23
ATOM	1673	NZ	LYS	1656	27.592	16.186	17.062	1.00	61.72
ATOM	1677	C	LYS	1656	20.777	14.560	14.855	1.00	68.73
ATOM	1678	O	LYS	1656	19.695	15.148	14.837	1.00	69.20
ATOM	1679	N	THR	1657	20.928	13.337	15.359	1.00	68.48
ATOM	1681	CA	THR	1657	19.821	12.607	15.960	1.00	67.93
ATOM	1682	CB	THR	1657	20.109	11.078	16.021	1.00	68.93
ATOM	1683	OG1	THR	1657	21.295	10.823	16.787	1.00	68.72
ATOM	1685	CG2	THR	1657	20.289	10.500	14.637	1.00	68.83
ATOM	1686	C	THR	1657	19.682	13.131	17.383	1.00	67.80
ATOM	1687	O	THR	1657	20.424	14.022	17.790	1.00	67.87
ATOM	1688	N	ALA	1658	18.753	12.569	18.148	1.00	68.95
ATOM	1690	CA	ALA	1658	18.580	12.992	19.537	1.00	70.64
ATOM	1691	CB	ALA	1658	17.391	12.254	20.173	1.00	71.19
ATOM	1692	C	ALA	1658	19.880	12.709	20.313	1.00	69.64
ATOM	1693	O	ALA	1658	20.394	13.566	21.042	1.00	70.13
ATOM	1694	N	ASN	1659	20.440	11.526	20.080	1.00	68.02
ATOM	1696	CA	ASN	1659	21.663	11.092	20.746	1.00	66.10
ATOM	1697	CB	ASN	1659	21.835	9.583	20.557	1.00	70.23
ATOM	1698	CG	ASN	1659	22.632	8.937	21.679	1.00	74.09
ATOM	1699	OD1	ASN	1659	22.525	9.331	22.840	1.00	75.21
ATOM	1700	ND2	ASN	1659	23.402	7.907	21.342	1.00	75.03
ATOM	1703	C	ASN	1659	22.910	11.816	20.249	1.00	63.30
ATOM	1704	O	ASN	1659	24.004	11.585	20.762	1.00	61.12
ATOM	1705	N	GLY	1660	22.744	12.678	19.246	1.00	61.61
ATOM	1707	CA	GLY	1660	23.867	13.421	18.689	1.00	59.06
ATOM	1708	C	GLY	1660	24.604	12.750	17.536	1.00	56.84
ATOM	1709	O	GLY	1660	25.726	13.132	17.196	1.00	55.69
ATOM	1710	N	ARG	1661	23.980	11.758	16.914	1.00	55.73
ATOM	1712	CA	ARG	1661	24.626	11.062	15.808	1.00	52.76
ATOM	1713	CB	ARG	1661	24.387	9.549	15.883	1.00	52.39
ATOM	1714	CG	ARG	1661	24.977	8.874	17.111	1.00	54.08
ATOM	1715	CD	ARG	1661	24.776	7.376	17.045	1.00	58.37
ATOM	1716	NE	ARG	1661	25.178	6.665	18.260	1.00	59.27
ATOM	1718	CZ	ARG	1661	24.952	5.369	18.471	1.00	59.83
ATOM	1719	NH1	ARG	1661	24.319	4.643	17.550	1.00	57.04
ATOM	1722	NH2	ARG	1661	25.375	4.792	19.591	1.00	59.47

ATOM	1725	C	ARG	1661	24.167	11.609	14.468	1.00	49.58
ATOM	1726	O	ARG	1661	23.169	12.321	14.375	1.00	47.38
ATOM	1727	N	LEU	1662	24.911	11.266	13.430	1.00	46.26
ATOM	1729	CA	LEU	1662	24.600	11.717	12.092	1.00	44.75
ATOM	1730	CB	LEU	1662	25.871	12.261	11.425	1.00	43.49
ATOM	1731	CG	LEU	1662	26.430	13.561	12.020	1.00	43.01
ATOM	1732	CD1	LEU	1662	27.918	13.705	11.727	1.00	42.40
ATOM	1733	CD2	LEU	1662	25.644	14.760	11.507	1.00	40.19
ATOM	1734	C	LEU	1662	23.999	10.570	11.276	1.00	43.58
ATOM	1735	O	LEU	1662	24.704	9.628	10.892	1.00	43.68
ATOM	1736	N	PRO	1663	22.680	10.631	11.010	1.00	40.72
ATOM	1737	CD	PRO	1663	21.723	11.629	11.521	1.00	40.27
ATOM	1738	CA	PRO	1663	21.981	9.603	10.237	1.00	36.86
ATOM	1739	CB	PRO	1663	20.595	10.214	10.035	1.00	36.67
ATOM	1740	CG	PRO	1663	20.375	10.937	11.314	1.00	36.84
ATOM	1741	C	PRO	1663	22.640	9.266	8.907	1.00	33.34
ATOM	1742	O	PRO	1663	22.442	8.161	8.401	1.00	33.65
ATOM	1743	N	VAL	1664	23.427	10.188	8.343	1.00	31.26
ATOM	1745	CA	VAL	1664	24.095	9.915	7.058	1.00	30.43
ATOM	1746	CB	VAL	1664	24.887	11.125	6.466	1.00	27.09
ATOM	1747	CG1	VAL	1664	23.947	12.199	6.040	1.00	23.98
ATOM	1748	CG2	VAL	1664	25.894	11.654	7.464	1.00	26.06
ATOM	1749	C	VAL	1664	25.044	8.728	7.163	1.00	28.18
ATOM	1750	O	VAL	1664	25.461	8.178	6.153	1.00	28.30
ATOM	1751	N	LYS	1665	25.353	8.326	8.389	1.00	25.52
ATOM	1753	CA	LYS	1665	26.243	7.200	8.612	1.00	25.48
ATOM	1754	CB	LYS	1665	26.915	7.334	9.979	1.00	23.52
ATOM	1755	CG	LYS	1665	27.910	8.452	10.001	1.00	23.14
ATOM	1756	CD	LYS	1665	28.363	8.776	11.400	1.00	29.84
ATOM	1757	CE	LYS	1665	29.430	9.871	11.385	1.00	28.33
ATOM	1758	NZ	LYS	1665	29.794	10.283	12.777	1.00	30.88
ATOM	1762	C	LYS	1665	25.595	5.823	8.413	1.00	25.26
ATOM	1763	O	LYS	1665	26.261	4.798	8.512	1.00	23.05
ATOM	1764	N	TRP	1666	24.289	5.815	8.156	1.00	27.05
ATOM	1766	CA	TRP	1666	23.543	4.588	7.884	1.00	27.17
ATOM	1767	CB	TRP	1666	22.282	4.529	8.760	1.00	26.98
ATOM	1768	CG	TRP	1666	22.563	4.067	10.197	1.00	29.62
ATOM	1769	CD2	TRP	1666	23.065	4.857	11.283	1.00	29.64
ATOM	1770	CE2	TRP	1666	23.230	3.988	12.393	1.00	28.25
ATOM	1771	CE3	TRP	1666	23.406	6.208	11.430	1.00	29.15
ATOM	1772	CD1	TRP	1666	22.436	2.793	10.690	1.00	26.48
ATOM	1773	NE1	TRP	1666	22.834	2.737	11.997	1.00	24.81
ATOM	1775	CZ2	TRP	1666	23.719	4.430	13.636	1.00	28.40
ATOM	1776	CZ3	TRP	1666	23.894	6.647	12.670	1.00	29.38
ATOM	1777	CH2	TRP	1666	24.048	5.756	13.749	1.00	29.83
ATOM	1778	C	TRP	1666	23.176	4.499	6.385	1.00	27.71
ATOM	1779	O	TRP	1666	22.745	3.451	5.900	1.00	29.42
ATOM	1780	N	MET	1667	23.439	5.572	5.645	1.00	25.52
ATOM	1782	CA	MET	1667	23.098	5.642	4.232	1.00	25.24
ATOM	1783	CB	MET	1667	22.972	7.095	3.792	1.00	26.58
ATOM	1784	CG	MET	1667	21.830	7.836	4.391	1.00	32.35
ATOM	1785	SD	MET	1667	21.846	9.559	3.877	1.00	40.32

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ATOM	1786	CE	MET	1667	21.033	9.447	2.341	1.00	38.17
ATOM	1787	C	MET	1667	24.042	4.960	3.276	1.00	25.07
ATOM	1788	O	MET	1667	25.256	5.037	3.411	1.00	27.61
ATOM	1789	N	ALA	1668	23.473	4.302	2.282	1.00	24.92
ATOM	1791	CA	ALA	1668	24.272	3.647	1.271	1.00	26.92
ATOM	1792	CB	ALA	1668	23.397	2.720	0.425	1.00	25.09
ATOM	1793	C	ALA	1668	24.866	4.759	0.410	1.00	27.82
ATOM	1794	O	ALA	1668	24.254	5.817	0.242	1.00	27.06
ATOM	1795	N	PRO	1669	26.050	4.530	-0.170	1.00	27.84
ATOM	1796	CD	PRO	1669	26.912	3.339	-0.107	1.00	27.12
ATOM	1797	CA	PRO	1669	26.662	5.561	-1.005	1.00	28.04
ATOM	1798	CB	PRO	1669	27.868	4.835	-1.593	1.00	26.71
ATOM	1799	CG	PRO	1669	28.249	3.893	-0.498	1.00	27.49
ATOM	1800	C	PRO	1669	25.734	6.078	-2.108	1.00	28.51
ATOM	1801	O	PRO	1669	25.685	7.281	-2.371	1.00	30.64
ATOM	1802	N	GLU	1670	24.992	5.179	-2.746	1.00	28.25
ATOM	1804	CA	GLU	1670	24.095	5.584	-3.826	1.00	26.82
ATOM	1805	CB	GLU	1670	23.600	4.369	-4.620	1.00	29.32
ATOM	1806	CG	GLU	1670	22.604	3.486	-3.889	1.00	30.38
ATOM	1807	CD	GLU	1670	23.223	2.266	-3.229	1.00	32.52
ATOM	1808	OE1	GLU	1670	22.444	1.393	-2.794	1.00	28.06
ATOM	1809	OE2	GLU	1670	24.474	2.175	-3.130	1.00	28.67
ATOM	1810	C	GLU	1670	22.924	6.440	-3.356	1.00	24.79
ATOM	1811	O	GLU	1670	22.410	7.236	-4.123	1.00	22.31
ATOM	1812	N	ALA	1671	22.512	6.265	-2.101	1.00	26.70
ATOM	1814	CA	ALA	1671	21.423	7.040	-1.490	1.00	25.67
ATOM	1815	CB	ALA	1671	20.813	6.292	-0.312	1.00	18.88
ATOM	1816	C	ALA	1671	21.984	8.365	-1.006	1.00	26.05
ATOM	1817	O	ALA	1671	21.400	9.414	-1.229	1.00	28.14
ATOM	1818	N	LEU	1672	23.138	8.300	-0.358	1.00	29.03
ATOM	1820	CA	LEU	1672	23.807	9.481	0.172	1.00	34.07
ATOM	1821	CB	LEU	1672	25.030	9.064	0.986	1.00	34.45
ATOM	1822	CG	LEU	1672	25.870	10.157	1.648	1.00	39.50
ATOM	1823	CD1	LEU	1672	25.081	10.853	2.740	1.00	41.71
ATOM	1824	CD2	LEU	1672	27.123	9.530	2.243	1.00	40.16
ATOM	1825	C	LEU	1672	24.248	10.431	-0.942	1.00	38.47
ATOM	1826	O	LEU	1672	23.958	11.625	-0.898	1.00	42.25
ATOM	1827	N	PHE	1673	24.924	9.901	-1.956	1.00	39.07
ATOM	1829	CA	PHE	1673	25.414	10.725	-3.053	1.00	38.00
ATOM	1830	CB	PHE	1673	26.699	10.110	-3.639	1.00	36.48
ATOM	1831	CG	PHE	1673	27.826	9.928	-2.637	1.00	33.36
ATOM	1832	CD1	PHE	1673	28.524	8.724	-2.580	1.00	29.55
ATOM	1833	CD2	PHE	1673	28.205	10.960	-1.779	1.00	31.85
ATOM	1834	CE1	PHE	1673	29.580	8.540	-1.692	1.00	26.33
ATOM	1835	CE2	PHE	1673	29.265	10.786	-0.880	1.00	30.95
ATOM	1836	CZ	PHE	1673	29.954	9.568	-0.838	1.00	28.99
ATOM	1837	C	PHE	1673	24.413	10.957	-4.194	1.00	39.64
ATOM	1838	O	PHE	1673	24.364	12.046	-4.760	1.00	37.72
ATOM	1839	N	ASP	1674	23.651	9.928	-4.554	1.00	41.35
ATOM	1841	CA	ASP	1674	22.716	10.027	-5.666	1.00	43.38
ATOM	1842	CB	ASP	1674	22.934	8.858	-6.625	1.00	47.84
ATOM	1843	CG	ASP	1674	24.359	8.765	-7.121	1.00	53.24

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ATOM	1844	OD1	ASP	1674	25.049	9.808	-7.172	1.00	56.20
ATOM	1845	OD2	ASP	1674	24.786	7.640	-7.460	1.00	55.73
ATOM	1846	C	ASP	1674	21.239	10.083	-5.321	1.00	45.94
ATOM	1847	O	ASP	1674	20.402	10.200	-6.222	1.00	47.80
ATOM	1848	N	ARG	1675	20.903	9.953	-4.040	1.00	45.98
ATOM	1850	CA	ARG	1675	19.503	9.981	-3.608	1.00	43.76
ATOM	1851	CB	ARG	1675	18.872	11.346	-3.887	1.00	48.61
ATOM	1852	CG	ARG	1675	19.519	12.478	-3.142	1.00	58.37
ATOM	1853	CD	ARG	1675	19.468	13.715	-3.992	1.00	70.39
ATOM	1854	NE	ARG	1675	20.035	14.867	-3.306	1.00	79.14
ATOM	1856	CZ	ARG	1675	19.612	16.116	-3.472	1.00	82.95
ATOM	1857	NH1	ARG	1675	18.610	16.386	-4.308	1.00	82.00
ATOM	1860	NH2	ARG	1675	20.194	17.097	-2.793	1.00	87.42
ATOM	1863	C	ARG	1675	18.647	8.882	-4.236	1.00	39.26
ATOM	1864	O	ARG	1675	17.461	9.074	-4.488	1.00	37.29
ATOM	1865	N	ILE	1676	19.270	7.746	-4.526	1.00	35.86
ATOM	1867	CA	ILE	1676	18.544	6.614	-5.081	1.00	32.76
ATOM	1868	CB	ILE	1676	19.324	5.927	-6.192	1.00	31.73
ATOM	1869	CG2	ILE	1676	18.450	4.902	-6.868	1.00	30.02
ATOM	1870	CG1	ILE	1676	19.767	6.955	-7.219	1.00	32.68
ATOM	1871	CD1	ILE	1676	20.658	6.371	-8.272	1.00	35.75
ATOM	1872	C	ILE	1676	18.329	5.625	-3.946	1.00	31.08
ATOM	1873	O	ILE	1676	19.264	4.962	-3.505	1.00	28.77
ATOM	1874	N	TYR	1677	17.102	5.558	-3.444	1.00	30.32
ATOM	1876	CA	TYR	1677	16.779	4.653	-2.348	1.00	29.68
ATOM	1877	CB	TYR	1677	15.846	5.329	-1.354	1.00	31.14
ATOM	1878	CG	TYR	1677	16.523	6.395	-0.514	1.00	32.95
ATOM	1879	CD1	TYR	1677	16.616	7.721	-0.958	1.00	30.40
ATOM	1880	CE1	TYR	1677	17.208	8.707	-0.171	1.00	27.57
ATOM	1881	CD2	TYR	1677	17.048	6.082	0.743	1.00	32.13
ATOM	1882	CE2	TYR	1677	17.642	7.059	1.543	1.00	31.50
ATOM	1883	CZ	TYR	1677	17.711	8.366	1.081	1.00	31.12
ATOM	1884	OH	TYR	1677	18.235	9.326	1.912	1.00	32.18
ATOM	1886	C	TYR	1677	16.123	3.424	-2.933	1.00	28.88
ATOM	1887	O	TYR	1677	15.268	3.537	-3.811	1.00	32.20
ATOM	1888	N	THR	1678	16.556	2.253	-2.481	1.00	26.34
ATOM	1890	CA	THR	1678	16.023	0.988	-2.971	1.00	25.55
ATOM	1891	CB	THR	1678	16.917	0.394	-4.043	1.00	28.81
ATOM	1892	OG1	THR	1678	18.221	0.179	-3.483	1.00	34.06
ATOM	1894	CG2	THR	1678	17.010	1.320	-5.267	1.00	27.25
ATOM	1895	C	THR	1678	16.037	0.007	-1.827	1.00	21.78
ATOM	1896	O	THR	1678	16.505	0.312	-0.744	1.00	25.57
ATOM	1897	N	HIS	1679	15.559	-1.198	-2.071	1.00	20.86
ATOM	1899	CA	HIS	1679	15.580	-2.216	-1.030	1.00	20.30
ATOM	1900	CB	HIS	1679	14.816	-3.453	-1.499	1.00	17.22
ATOM	1901	CG	HIS	1679	13.367	-3.196	-1.797	1.00	19.02
ATOM	1902	CD2	HIS	1679	12.662	-3.275	-2.958	1.00	14.89
ATOM	1903	ND1	HIS	1679	12.459	-2.830	-0.826	1.00	18.98
ATOM	1905	CE1	HIS	1679	11.260	-2.697	-1.370	1.00	16.10
ATOM	1906	NE2	HIS	1679	11.359	-2.961	-2.663	1.00	15.18
ATOM	1908	C	HIS	1679	17.050	-2.535	-0.761	1.00	20.44
ATOM	1909	O	HIS	1679	17.428	-2.901	0.356	1.00	22.58

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ATOM	1910	N	GLN	1680	17.874	-2.310	-1.781	1.00	20.58
ATOM	1912	CA	GLN	1680	19.303	-2.539	-1.721	1.00	22.70
ATOM	1913	CB	GLN	1680	19.935	-2.427	-3.106	1.00	26.26
ATOM	1914	CG	GLN	1680	19.934	-3.711	-3.889	1.00	31.86
ATOM	1915	CD	GLN	1680	18.949	-3.687	-5.026	1.00	37.54
ATOM	1916	OE1	GLN	1680	17.931	-3.000	-4.961	1.00	42.70
ATOM	1917	NE2	GLN	1680	19.256	-4.409	-6.091	1.00	37.42
ATOM	1920	C	GLN	1680	19.985	-1.559	-0.797	1.00	24.93
ATOM	1921	O	GLN	1680	20.875	-1.943	-0.039	1.00	26.39
ATOM	1922	N	SER	1681	19.605	-0.286	-0.867	1.00	24.70
ATOM	1924	CA	SER	1681	20.239	0.678	0.030	1.00	23.24
ATOM	1925	CB	SER	1681	19.923	2.128	-0.346	1.00	19.33
ATOM	1926	OG	SER	1681	18.544	2.326	-0.545	1.00	18.55
ATOM	1928	C	SER	1681	19.852	0.364	1.464	1.00	21.77
ATOM	1929	O	SER	1681	20.645	0.609	2.366	1.00	24.14
ATOM	1930	N	ASP	1682	18.659	-0.210	1.670	1.00	21.80
ATOM	1932	CA	ASP	1682	18.180	-0.604	3.003	1.00	22.45
ATOM	1933	CB	ASP	1682	16.730	-1.111	2.963	1.00	25.27
ATOM	1934	CG	ASP	1682	15.678	0.004	3.132	1.00	28.21
ATOM	1935	OD1	ASP	1682	14.500	-0.245	2.786	1.00	25.41
ATOM	1936	OD2	ASP	1682	15.992	1.102	3.639	1.00	30.19
ATOM	1937	C	ASP	1682	19.076	-1.736	3.517	1.00	23.69
ATOM	1938	O	ASP	1682	19.385	-1.799	4.709	1.00	24.74
ATOM	1939	N	VAL	1683	19.474	-2.635	2.620	1.00	23.49
ATOM	1941	CA	VAL	1683	20.354	-3.737	3.003	1.00	21.77
ATOM	1942	CB	VAL	1683	20.543	-4.741	1.837	1.00	20.49
ATOM	1943	CG1	VAL	1683	21.770	-5.613	2.039	1.00	19.82
ATOM	1944	CG2	VAL	1683	19.320	-5.618	1.736	1.00	19.29
ATOM	1945	C	VAL	1683	21.674	-3.153	3.523	1.00	21.93
ATOM	1946	O	VAL	1683	22.161	-3.570	4.573	1.00	21.06
ATOM	1947	N	TRP	1684	22.207	-2.143	2.837	1.00	20.64
ATOM	1949	CA	TRP	1684	23.424	-1.482	3.295	1.00	20.98
ATOM	1950	CB	TRP	1684	23.711	-0.224	2.463	1.00	19.56
ATOM	1951	CG	TRP	1684	24.859	0.609	2.970	1.00	23.22
ATOM	1952	CD2	TRP	1684	26.182	0.686	2.421	1.00	24.64
ATOM	1953	CE2	TRP	1684	26.929	1.559	3.249	1.00	24.69
ATOM	1954	CE3	TRP	1684	26.813	0.102	1.315	1.00	26.41
ATOM	1955	CD1	TRP	1684	24.857	1.430	4.075	1.00	23.64
ATOM	1956	NE1	TRP	1684	26.097	1.994	4.246	1.00	23.28
ATOM	1958	CZ2	TRP	1684	28.275	1.859	3.000	1.00	20.55
ATOM	1959	CZ3	TRP	1684	28.165	0.409	1.072	1.00	22.82
ATOM	1960	CH2	TRP	1684	28.872	1.274	1.908	1.00	19.24
ATOM	1961	C	TRP	1684	23.201	-1.112	4.771	1.00	21.12
ATOM	1962	O	TRP	1684	23.931	-1.560	5.652	1.00	22.08
ATOM	1963	N	SER	1685	22.150	-0.342	5.032	1.00	23.27
ATOM	1965	CA	SER	1685	21.787	0.086	6.386	1.00	22.54
ATOM	1966	CB	SER	1685	20.429	0.768	6.356	1.00	21.98
ATOM	1967	OG	SER	1685	20.318	1.626	5.220	1.00	25.48
ATOM	1969	C	SER	1685	21.747	-1.068	7.389	1.00	21.33
ATOM	1970	O	SER	1685	22.145	-0.902	8.545	1.00	19.52
ATOM	1971	N	PHE	1686	21.260	-2.228	6.946	1.00	23.10
ATOM	1973	CA	PHE	1686	21.174	-3.424	7.800	1.00	23.09

ATOM	1974	CB	PHE	1686	20.409	-4.550	7.095	1.00	22.77
ATOM	1975	CG	PHE	1686	20.192	-5.767	7.962	1.00	25.82
ATOM	1976	CD1	PHE	1686	19.378	-5.694	9.096	1.00	25.54
ATOM	1977	CD2	PHE	1686	20.808	-6.987	7.649	1.00	23.88
ATOM	1978	CE1	PHE	1686	19.185	-6.809	9.913	1.00	24.25
ATOM	1979	CE2	PHE	1686	20.622	-8.109	8.455	1.00	22.67
ATOM	1980	CZ	PHE	1686	19.809	-8.023	9.585	1.00	26.30
ATOM	1981	C	PHE	1686	22.569	-3.919	8.240	1.00	21.77
ATOM	1982	O	PHE	1686	22.739	-4.450	9.350	1.00	20.47
ATOM	1983	N	GLY	1687	23.553	-3.773	7.358	1.00	20.63
ATOM	1985	CA	GLY	1687	24.913	-4.163	7.685	1.00	19.29
ATOM	1986	C	GLY	1687	25.407	-3.276	8.822	1.00	21.64
ATOM	1987	O	GLY	1687	26.094	-3.755	9.727	1.00	19.46
ATOM	1988	N	VAL	1688	25.008	-1.996	8.794	1.00	22.19
ATOM	1990	CA	VAL	1688	25.372	-1.024	9.831	1.00	21.99
ATOM	1991	CB	VAL	1688	25.048	0.458	9.423	1.00	23.20
ATOM	1992	CG1	VAL	1688	25.439	1.424	10.540	1.00	21.22
ATOM	1993	CG2	VAL	1688	25.820	0.846	8.161	1.00	21.25
ATOM	1994	C	VAL	1688	24.621	-1.403	11.100	1.00	23.33
ATOM	1995	O	VAL	1688	25.204	-1.420	12.187	1.00	24.98
ATOM	1996	N	LEU	1689	23.339	-1.734	10.969	1.00	24.36
ATOM	1998	CA	LEU	1689	22.542	-2.161	12.122	1.00	23.92
ATOM	1999	CB	LEU	1689	21.072	-2.392	11.714	1.00	22.57
ATOM	2000	CG	LEU	1689	19.981	-2.427	12.805	1.00	23.41
ATOM	2001	CD1	LEU	1689	18.614	-2.295	12.164	1.00	19.14
ATOM	2002	CD2	LEU	1689	20.048	-3.700	13.658	1.00	22.75
ATOM	2003	C	LEU	1689	23.158	-3.447	12.717	1.00	25.22
ATOM	2004	O	LEU	1689	23.202	-3.592	13.937	1.00	25.58
ATOM	2005	N	LEU	1690	23.614	-4.379	11.871	1.00	25.47
ATOM	2007	CA	LEU	1690	24.256	-5.604	12.376	1.00	26.26
ATOM	2008	CB	LEU	1690	24.730	-6.531	11.255	1.00	26.22
ATOM	2009	CG	LEU	1690	23.809	-7.501	10.515	1.00	26.21
ATOM	2010	CD1	LEU	1690	24.662	-8.259	9.523	1.00	25.45
ATOM	2011	CD2	LEU	1690	23.135	-8.487	11.458	1.00	21.17
ATOM	2012	C	LEU	1690	25.471	-5.204	13.189	1.00	26.51
ATOM	2013	O	LEU	1690	25.710	-5.747	14.273	1.00	29.07
ATOM	2014	N	TRP	1691	26.240	-4.255	12.660	1.00	26.26
ATOM	2016	CA	TRP	1691	27.431	-3.761	13.341	1.00	25.08
ATOM	2017	CB	TRP	1691	28.129	-2.706	12.493	1.00	25.16
ATOM	2018	CG	TRP	1691	29.456	-2.268	13.039	1.00	27.49
ATOM	2019	CD2	TRP	1691	29.701	-1.163	13.925	1.00	25.81
ATOM	2020	CE2	TRP	1691	31.100	-1.070	14.103	1.00	22.63
ATOM	2021	CE3	TRP	1691	28.870	-0.236	14.575	1.00	26.70
ATOM	2022	CD1	TRP	1691	30.688	-2.798	12.735	1.00	23.03
ATOM	2023	NE1	TRP	1691	31.675	-2.078	13.371	1.00	25.19
ATOM	2025	CZ2	TRP	1691	31.690	-0.085	14.900	1.00	18.66
ATOM	2026	CZ3	TRP	1691	29.459	0.745	15.371	1.00	25.66
ATOM	2027	CH2	TRP	1691	30.861	0.812	15.523	1.00	23.00
ATOM	2028	C	TRP	1691	27.114	-3.195	14.727	1.00	24.63
ATOM	2029	O	TRP	1691	27.871	-3.393	15.662	1.00	27.79
ATOM	2030	N	GLU	1692	25.985	-2.506	14.862	1.00	26.48
ATOM	2032	CA	GLU	1692	25.574	-1.938	16.155	1.00	24.98

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ATOM	2033	CB	GLU	1692	24.335	-1.060	15.994	1.00	22.29
ATOM	2034	CG	GLU	1692	24.507	0.107	15.056	1.00	18.31
ATOM	2035	CD	GLU	1692	23.255	0.933	14.978	1.00	25.10
ATOM	2036	OE1	GLU	1692	22.433	0.704	14.066	1.00	26.95
ATOM	2037	OE2	GLU	1692	23.067	1.815	15.840	1.00	27.05
ATOM	2038	C	GLU	1692	25.260	-3.036	17.163	1.00	25.18
ATOM	2039	O	GLU	1692	25.602	-2.927	18.341	1.00	26.12
ATOM	2040	N	ILE	1693	24.593	-4.087	16.698	1.00	27.16
ATOM	2042	CA	ILE	1693	24.231	-5.214	17.555	1.00	25.91
ATOM	2043	CB	ILE	1693	23.373	-6.287	16.777	1.00	25.70
ATOM	2044	CG2	ILE	1693	23.171	-7.564	17.638	1.00	18.73
ATOM	2045	CG1	ILE	1693	22.005	-5.682	16.382	1.00	23.45
ATOM	2046	CD1	ILE	1693	21.208	-6.485	15.346	1.00	15.62
ATOM	2047	C	ILE	1693	25.496	-5.847	18.107	1.00	26.70
ATOM	2048	O	ILE	1693	25.672	-5.961	19.316	1.00	28.19
ATOM	2049	N	PHE	1694	26.442	-6.133	17.229	1.00	28.78
ATOM	2051	CA	PHE	1694	27.664	-6.779	17.679	1.00	29.72
ATOM	2052	CB	PHE	1694	28.261	-7.598	16.542	1.00	27.18
ATOM	2053	CG	PHE	1694	27.315	-8.649	16.048	1.00	25.38
ATOM	2054	CD1	PHE	1694	26.793	-8.599	14.770	1.00	26.16
ATOM	2055	CD2	PHE	1694	26.844	-9.625	16.919	1.00	26.37
ATOM	2056	CE1	PHE	1694	25.808	-9.505	14.370	1.00	31.37
ATOM	2057	CE2	PHE	1694	25.863	-10.533	16.536	1.00	25.23
ATOM	2058	CZ	PHE	1694	25.337	-10.478	15.268	1.00	29.46
ATOM	2059	C	PHE	1694	28.663	-5.906	18.438	1.00	30.92
ATOM	2060	O	PHE	1694	29.697	-6.403	18.902	1.00	32.23
ATOM	2061	N	THR	1695	28.344	-4.616	18.575	1.00	29.46
ATOM	2063	CA	THR	1695	29.170	-3.698	19.348	1.00	27.17
ATOM	2064	CB	THR	1695	29.665	-2.474	18.535	1.00	23.32
ATOM	2065	OG1	THR	1695	28.553	-1.710	18.046	1.00	24.73
ATOM	2067	CG2	THR	1695	30.538	-2.914	17.395	1.00	21.34
ATOM	2068	C	THR	1695	28.307	-3.230	20.519	1.00	28.81
ATOM	2069	O	THR	1695	28.707	-2.346	21.289	1.00	31.85
ATOM	2070	N	LEU	1696	27.130	-3.841	20.651	1.00	26.30
ATOM	2072	CA	LEU	1696	26.188	-3.523	21.720	1.00	25.99
ATOM	2073	CB	LEU	1696	26.704	-4.043	23.060	1.00	24.51
ATOM	2074	CG	LEU	1696	26.974	-5.539	23.194	1.00	23.32
ATOM	2075	CD1	LEU	1696	27.447	-5.843	24.597	1.00	26.45
ATOM	2076	CD2	LEU	1696	25.726	-6.297	22.907	1.00	29.79
ATOM	2077	C	LEU	1696	25.892	-2.036	21.837	1.00	24.90
ATOM	2078	O	LEU	1696	26.083	-1.457	22.889	1.00	28.99
ATOM	2079	N	GLY	1697	25.386	-1.432	20.771	1.00	25.05
ATOM	2081	CA	GLY	1697	25.072	-0.016	20.811	1.00	24.31
ATOM	2082	C	GLY	1697	26.241	0.847	20.381	1.00	27.15
ATOM	2083	O	GLY	1697	26.297	2.035	20.701	1.00	29.57
ATOM	2084	N	GLY	1698	27.177	0.261	19.639	1.00	27.33
ATOM	2086	CA	GLY	1698	28.319	1.023	19.178	1.00	27.04
ATOM	2087	C	GLY	1698	27.966	2.109	18.173	1.00	29.78
ATOM	2088	O	GLY	1698	27.115	1.929	17.301	1.00	32.03
ATOM	2089	N	SER	1699	28.633	3.247	18.295	1.00	30.60
ATOM	2091	CA	SER	1699	28.413	4.385	17.414	1.00	31.48
ATOM	2092	CB	SER	1699	28.747	5.692	18.164	1.00	32.97

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ATOM	2093	OG	SER	1699	28.350	6.848	17.436	1.00	37.75
ATOM	2095	C	SER	1699	29.323	4.239	16.188	1.00	32.74
ATOM	2096	O	SER	1699	30.541	4.034	16.321	1.00	33.04
ATOM	2097	N	PRO	1700	28.732	4.276	14.979	1.00	31.40
ATOM	2098	CD	PRO	1700	27.288	4.320	14.688	1.00	30.88
ATOM	2099	CA	PRO	1700	29.507	4.153	13.737	1.00	30.55
ATOM	2100	CB	PRO	1700	28.420	4.024	12.657	1.00	30.13
ATOM	2101	CG	PRO	1700	27.228	3.535	13.398	1.00	31.10
ATOM	2102	C	PRO	1700	30.300	5.427	13.509	1.00	31.19
ATOM	2103	O	PRO	1700	29.766	6.522	13.651	1.00	35.48
ATOM	2104	N	TYR	1701	31.574	5.277	13.175	1.00	29.51
ATOM	2106	CA	TYR	1701	32.446	6.412	12.899	1.00	30.10
ATOM	2107	CB	TYR	1701	32.084	7.029	11.541	1.00	32.84
ATOM	2108	CG	TYR	1701	32.102	6.078	10.353	1.00	38.43
ATOM	2109	CD1	TYR	1701	30.921	5.795	9.643	1.00	40.14
ATOM	2110	CE1	TYR	1701	30.930	5.000	8.513	1.00	39.07
ATOM	2111	CD2	TYR	1701	33.298	5.522	9.890	1.00	38.19
ATOM	2112	CE2	TYR	1701	33.320	4.726	8.754	1.00	41.52
ATOM	2113	CZ	TYR	1701	32.134	4.471	8.067	1.00	44.97
ATOM	2114	OH	TYR	1701	32.151	3.700	6.919	1.00	54.77
ATOM	2116	C	TYR	1701	32.426	7.524	13.965	1.00	30.38
ATOM	2117	O	TYR	1701	32.009	8.655	13.685	1.00	30.54
ATOM	2118	N	PRO	1702	32.947	7.239	15.170	1.00	30.61
ATOM	2119	CD	PRO	1702	33.578	5.985	15.608	1.00	29.72
ATOM	2120	CA	PRO	1702	32.971	8.239	16.248	1.00	28.48
ATOM	2121	CB	PRO	1702	33.554	7.463	17.429	1.00	28.43
ATOM	2122	CG	PRO	1702	33.320	6.025	17.085	1.00	30.63
ATOM	2123	C	PRO	1702	33.897	9.385	15.981	1.00	26.93
ATOM	2124	O	PRO	1702	34.998	9.156	15.418	1.00	26.21
ATOM	2125	N	GLY	1703	33.440	10.613	16.084	1.00	29.51
ATOM	2127	CA	GLY	1703	34.239	11.787	15.767	1.00	28.57
ATOM	2128	C	GLY	1703	34.374	12.143	14.296	1.00	28.97
ATOM	2129	O	GLY	1703	35.055	13.104	13.962	1.00	29.54
ATOM	2130	N	VAL	1704	33.726	11.380	13.418	1.00	30.90
ATOM	2132	CA	VAL	1704	33.798	11.616	11.975	1.00	29.48
ATOM	2133	CB	VAL	1704	33.806	10.289	11.228	1.00	28.23
ATOM	2134	CG1	VAL	1704	34.074	10.525	9.750	1.00	31.57
ATOM	2135	CG2	VAL	1704	34.851	9.375	11.822	1.00	28.40
ATOM	2136	C	VAL	1704	32.620	12.466	11.477	1.00	33.14
ATOM	2137	O	VAL	1704	31.466	12.045	11.529	1.00	35.67
ATOM	2138	N	PRO	1705	32.906	13.681	10.979	1.00	35.22
ATOM	2139	CD	PRO	1705	34.217	14.348	11.008	1.00	38.03
ATOM	2140	CA	PRO	1705	31.868	14.587	10.474	1.00	35.96
ATOM	2141	CB	PRO	1705	32.534	15.953	10.627	1.00	35.84
ATOM	2142	CG	PRO	1705	33.939	15.661	10.279	1.00	37.29
ATOM	2143	C	PRO	1705	31.473	14.293	9.031	1.00	37.17
ATOM	2144	O	PRO	1705	32.255	13.690	8.288	1.00	38.39
ATOM	2145	N	VAL	1706	30.296	14.780	8.624	1.00	36.10
ATOM	2147	CA	VAL	1706	29.743	14.582	7.276	1.00	37.10
ATOM	2148	CB	VAL	1706	28.667	15.658	6.942	1.00	38.36
ATOM	2149	CG1	VAL	1706	28.106	15.441	5.535	1.00	38.93
ATOM	2150	CG2	VAL	1706	27.536	15.595	7.952	1.00	40.79

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ATOM	2151	C	VAL	1706	30.762	14.559	6.138	1.00	37.09
ATOM	2152	O	VAL	1706	30.927	13.543	5.461	1.00	38.75
ATOM	2153	N	GLU	1707	31.477	15.663	5.967	1.00	37.08
ATOM	2155	CA	GLU	1707	32.472	15.793	4.910	1.00	35.52
ATOM	2156	CB	GLU	1707	33.059	17.206	4.918	1.00	38.30
ATOM	2157	C	GLU	1707	33.588	14.762	4.945	1.00	34.20
ATOM	2158	O	GLU	1707	34.153	14.445	3.908	1.00	33.48
ATOM	2159	N	GLU	1708	33.936	14.273	6.132	1.00	34.20
ATOM	2161	CA	GLU	1708	34.981	13.256	6.241	1.00	36.08
ATOM	2162	CB	GLU	1708	35.555	13.178	7.660	1.00	40.39
ATOM	2163	CG	GLU	1708	36.212	14.464	8.179	1.00	45.41
ATOM	2164	CD	GLU	1708	37.471	14.871	7.430	1.00	50.66
ATOM	2165	OE1	GLU	1708	38.199	13.986	6.909	1.00	54.73
ATOM	2166	OE2	GLU	1708	37.747	16.092	7.392	1.00	52.85
ATOM	2167	C	GLU	1708	34.369	11.911	5.855	1.00	35.22
ATOM	2168	O	GLU	1708	35.035	11.045	5.260	1.00	34.04
ATOM	2169	N	LEU	1709	33.089	11.749	6.178	1.00	33.30
ATOM	2171	CA	LEU	1709	32.376	10.519	5.860	1.00	31.44
ATOM	2172	CB	LEU	1709	30.975	10.531	6.474	1.00	26.89
ATOM	2173	CG	LEU	1709	30.065	9.366	6.073	1.00	26.05
ATOM	2174	CD1	LEU	1709	30.652	8.036	6.503	1.00	22.75
ATOM	2175	CD2	LEU	1709	28.717	9.574	6.697	1.00	26.15
ATOM	2176	C	LEU	1709	32.291	10.325	4.350	1.00	31.18
ATOM	2177	O	LEU	1709	32.490	9.209	3.858	1.00	29.88
ATOM	2178	N	PHE	1710	32.011	11.408	3.623	1.00	30.16
ATOM	2180	CA	PHE	1710	31.915	11.333	2.169	1.00	31.64
ATOM	2181	CB	PHE	1710	31.658	12.710	1.567	1.00	33.44
ATOM	2182	CG	PHE	1710	30.287	13.231	1.827	1.00	37.78
ATOM	2183	CD1	PHE	1710	29.287	12.395	2.303	1.00	41.46
ATOM	2184	CD2	PHE	1710	29.991	14.565	1.613	1.00	40.72
ATOM	2185	CE1	PHE	1710	28.012	12.882	2.566	1.00	41.30
ATOM	2186	CE2	PHE	1710	28.715	15.058	1.875	1.00	42.99
ATOM	2187	CZ	PHE	1710	27.725	14.208	2.354	1.00	40.95
ATOM	2188	C	PHE	1710	33.202	10.771	1.609	1.00	32.38
ATOM	2189	O	PHE	1710	33.183	9.815	0.825	1.00	32.26
ATOM	2190	N	LYS	1711	34.310	11.336	2.085	1.00	31.26
ATOM	2192	CA	LYS	1711	35.664	10.971	1.697	1.00	29.73
ATOM	2193	CB	LYS	1711	36.642	11.932	2.379	1.00	33.49
ATOM	2194	CG	LYS	1711	38.103	11.716	2.042	1.00	39.79
ATOM	2195	CD	LYS	1711	38.981	12.731	2.755	1.00	43.35
ATOM	2196	CE	LYS	1711	40.413	12.686	2.238	1.00	46.23
ATOM	2197	NZ	LYS	1711	41.116	11.422	2.600	1.00	53.67
ATOM	2201	C	LYS	1711	35.999	9.501	2.015	1.00	29.34
ATOM	2202	O	LYS	1711	36.670	8.836	1.231	1.00	28.77
ATOM	2203	N	LEU	1712	35.541	9.000	3.164	1.00	30.40
ATOM	2205	CA	LEU	1712	35.776	7.599	3.532	1.00	28.72
ATOM	2206	CB	LEU	1712	35.241	7.295	4.942	1.00	27.71
ATOM	2207	CG	LEU	1712	35.971	7.870	6.166	1.00	28.23
ATOM	2208	CD1	LEU	1712	35.186	7.593	7.440	1.00	20.80
ATOM	2209	CD2	LEU	1712	37.389	7.297	6.266	1.00	27.01
ATOM	2210	C	LEU	1712	35.022	6.738	2.530	1.00	30.03
ATOM	2211	O	LEU	1712	35.571	5.796	1.957	1.00	29.28

ATOM	2212	N	LEU	1713	33.752	7.073	2.325	1.00	31.98
ATOM	2214	CA	LEU	1713	32.904	6.339	1.403	1.00	34.30
ATOM	2215	CB	LEU	1713	31.467	6.872	1.447	1.00	37.65
ATOM	2216	CG	LEU	1713	30.663	6.450	2.686	1.00	37.06
ATOM	2217	CD1	LEU	1713	29.367	7.217	2.781	1.00	36.80
ATOM	2218	CD2	LEU	1713	30.399	4.950	2.641	1.00	37.02
ATOM	2219	C	LEU	1713	33.451	6.344	-0.011	1.00	35.45
ATOM	2220	O	LEU	1713	33.468	5.298	-0.662	1.00	38.18
ATOM	2221	N	LYS	1714	33.920	7.498	-0.481	1.00	33.22
ATOM	2223	CA	LYS	1714	34.487	7.590	-1.821	1.00	31.46
ATOM	2224	CB	LYS	1714	34.881	9.027	-2.158	1.00	31.32
ATOM	2225	CG	LYS	1714	33.724	9.962	-2.399	1.00	33.49
ATOM	2226	CD	LYS	1714	32.814	9.439	-3.491	1.00	39.40
ATOM	2227	CE	LYS	1714	31.613	10.364	-3.720	1.00	44.79
ATOM	2228	NZ	LYS	1714	30.674	9.841	-4.771	1.00	50.41
ATOM	2232	C	LYS	1714	35.706	6.678	-1.953	1.00	32.53
ATOM	2233	O	LYS	1714	35.998	6.155	-3.025	1.00	35.46
ATOM	2234	N	GLU	1715	36.420	6.488	-0.856	1.00	33.50
ATOM	2236	CA	GLU	1715	37.602	5.644	-0.864	1.00	34.92
ATOM	2237	CB	GLU	1715	38.617	6.177	0.143	1.00	37.20
ATOM	2238	CG	GLU	1715	39.085	7.571	-0.221	1.00	44.59
ATOM	2239	CD	GLU	1715	39.654	8.372	0.946	1.00	51.44
ATOM	2240	OE1	GLU	1715	39.820	7.826	2.065	1.00	51.40
ATOM	2241	OE2	GLU	1715	39.930	9.573	0.726	1.00	54.23
ATOM	2242	C	GLU	1715	37.278	4.183	-0.581	1.00	35.09
ATOM	2243	O	GLU	1715	38.184	3.357	-0.482	1.00	37.59
ATOM	2244	N	GLY	1716	35.991	3.866	-0.455	1.00	33.79
ATOM	2246	CA	GLY	1716	35.576	2.498	-0.197	1.00	30.96
ATOM	2247	C	GLY	1716	35.852	1.976	1.198	1.00	29.06
ATOM	2248	O	GLY	1716	35.906	0.766	1.416	1.00	29.28
ATOM	2249	N	HIS	1717	35.995	2.879	2.155	1.00	28.16
ATOM	2251	CA	HIS	1717	36.282	2.489	3.532	1.00	29.80
ATOM	2252	CB	HIS	1717	36.534	3.743	4.378	1.00	33.13
ATOM	2253	CG	HIS	1717	36.794	3.469	5.826	1.00	36.22
ATOM	2254	CD2	HIS	1717	37.955	3.375	6.516	1.00	35.38
ATOM	2255	ND1	HIS	1717	35.782	3.279	6.746	1.00	37.81
ATOM	2257	CE1	HIS	1717	36.309	3.080	7.942	1.00	36.97
ATOM	2258	NE2	HIS	1717	37.624	3.134	7.830	1.00	35.83
ATOM	2260	C	HIS	1717	35.171	1.645	4.153	1.00	29.26
ATOM	2261	O	HIS	1717	33.987	1.900	3.940	1.00	31.43
ATOM	2262	N	ARG	1718	35.571	0.666	4.955	1.00	28.11
ATOM	2264	CA	ARG	1718	34.632	-0.212	5.640	1.00	30.67
ATOM	2265	CB	ARG	1718	34.592	-1.583	4.973	1.00	27.32
ATOM	2266	CG	ARG	1718	34.058	-1.586	3.557	1.00	28.77
ATOM	2267	CD	ARG	1718	32.609	-1.111	3.484	1.00	28.84
ATOM	2268	NE	ARG	1718	32.032	-1.167	2.131	1.00	24.96
ATOM	2270	CZ	ARG	1718	32.141	-0.206	1.204	1.00	23.90
ATOM	2271	NH1	ARG	1718	32.824	0.912	1.454	1.00	20.04
ATOM	2274	NH2	ARG	1718	31.513	-0.338	0.045	1.00	20.04
ATOM	2277	C	ARG	1718	35.091	-0.350	7.101	1.00	33.92
ATOM	2278	O	ARG	1718	36.300	-0.449	7.377	1.00	36.48
ATOM	2279	N	MET	1719	34.134	-0.355	8.028	1.00	33.22

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ATOM	2281	CA	MET	1719	34.428	-0.459	9.448	1.00	32.33
ATOM	2282	CB	MET	1719	33.148	-0.285	10.277	1.00	34.72
ATOM	2283	CG	MET	1719	32.454	1.066	10.076	1.00	35.04
ATOM	2284	SD	MET	1719	31.025	1.447	11.141	1.00	34.06
ATOM	2285	CE	MET	1719	29.757	0.470	10.409	1.00	33.14
ATOM	2286	C	MET	1719	35.068	-1.797	9.747	1.00	35.53
ATOM	2287	O	MET	1719	34.896	-2.756	8.991	1.00	35.48
ATOM	2288	N	ASP	1720	35.826	-1.843	10.840	1.00	38.65
ATOM	2290	CA	ASP	1720	36.521	-3.049	11.281	1.00	39.03
ATOM	2291	CB	ASP	1720	37.659	-2.678	12.237	1.00	43.11
ATOM	2292	CG	ASP	1720	38.743	-1.846	11.569	1.00	46.69
ATOM	2293	OD1	ASP	1720	38.587	-1.536	10.364	1.00	54.08
ATOM	2294	OD2	ASP	1720	39.750	-1.503	12.239	1.00	45.93
ATOM	2295	C	ASP	1720	35.580	-4.023	11.972	1.00	38.50
ATOM	2296	O	ASP	1720	34.554	-3.617	12.528	1.00	37.73
ATOM	2297	N	LYS	1721	35.961	-5.298	11.981	1.00	38.10
ATOM	2299	CA	LYS	1721	35.151	-6.339	12.600	1.00	38.12
ATOM	2300	CB	LYS	1721	35.727	-7.733	12.323	1.00	38.20
ATOM	2301	CG	LYS	1721	34.825	-8.858	12.825	1.00	38.48
ATOM	2302	CD	LYS	1721	35.375	-10.238	12.543	1.00	37.49
ATOM	2303	CE	LYS	1721	36.320	-10.691	13.625	1.00	39.11
ATOM	2304	NZ	LYS	1721	36.448	-12.167	13.628	1.00	40.75
ATOM	2308	C	LYS	1721	35.092	-6.142	14.091	1.00	40.24
ATOM	2309	O	LYS	1721	36.136	-6.032	14.739	1.00	42.70
ATOM	2310	N	PRO	1722	33.875	-6.082	14.658	1.00	41.23
ATOM	2311	CD	PRO	1722	32.547	-6.153	14.019	1.00	38.63
ATOM	2312	CA	PRO	1722	33.743	-5.901	16.104	1.00	41.71
ATOM	2313	CB	PRO	1722	32.223	-5.957	16.306	1.00	38.90
ATOM	2314	CG	PRO	1722	31.679	-5.442	15.016	1.00	34.19
ATOM	2315	C	PRO	1722	34.418	-7.079	16.819	1.00	43.96
ATOM	2316	O	PRO	1722	34.542	-8.174	16.250	1.00	43.02
ATOM	2317	N	SER	1723	34.915	-6.860	18.028	1.00	46.76
ATOM	2319	CA	SER	1723	35.493	-7.973	18.747	1.00	50.74
ATOM	2320	CB	SER	1723	36.265	-7.500	19.980	1.00	49.47
ATOM	2321	OG	SER	1723	35.400	-7.130	21.035	1.00	53.87
ATOM	2323	C	SER	1723	34.259	-8.782	19.143	1.00	53.24
ATOM	2324	O	SER	1723	33.136	-8.259	19.130	1.00	53.97
ATOM	2325	N	ASN	1724	34.443	-10.064	19.426	1.00	56.59
ATOM	2327	CA	ASN	1724	33.316	-10.899	19.825	1.00	59.55
ATOM	2328	CB	ASN	1724	32.739	-10.386	21.162	1.00	66.12
ATOM	2329	CG	ASN	1724	33.824	-10.128	22.213	1.00	71.34
ATOM	2330	OD1	ASN	1724	34.661	-10.990	22.485	1.00	73.38
ATOM	2331	ND2	ASN	1724	33.831	-8.926	22.779	1.00	74.19
ATOM	2334	C	ASN	1724	32.256	-10.900	18.711	1.00	57.31
ATOM	2335	O	ASN	1724	31.073	-10.662	18.940	1.00	59.27
ATOM	2336	N	CYS	1725	32.723	-11.132	17.493	1.00	54.50
ATOM	2338	CA	CYS	1725	31.881	-11.203	16.300	1.00	50.89
ATOM	2339	CB	CYS	1725	31.827	-9.848	15.576	1.00	50.09
ATOM	2340	SG	CYS	1725	30.893	-9.833	14.006	1.00	44.81
ATOM	2341	C	CYS	1725	32.596	-12.235	15.439	1.00	47.28
ATOM	2342	O	CYS	1725	33.820	-12.172	15.288	1.00	48.97
ATOM	2343	N	THR	1726	31.863	-13.229	14.950	1.00	42.60

ATOM	2345	CA	THR	1726	32.472	-14.275	14.139	1.00	39.22
ATOM	2346	CB	THR	1726	31.520	-15.494	13.984	1.00	36.36
ATOM	2347	OG1	THR	1726	30.290	-15.087	13.363	1.00	36.62
ATOM	2349	CG2	THR	1726	31.210	-16.084	15.326	1.00	33.12
ATOM	2350	C	THR	1726	32.858	-13.748	12.776	1.00	37.99
ATOM	2351	O	THR	1726	32.373	-12.704	12.357	1.00	39.57
ATOM	2352	N	ASN	1727	33.724	-14.473	12.080	1.00	37.02
ATOM	2354	CA	ASN	1727	34.133	-14.044	10.742	1.00	38.17
ATOM	2355	CB	ASN	1727	35.290	-14.880	10.221	1.00	40.63
ATOM	2356	CG	ASN	1727	36.580	-14.593	10.953	1.00	44.79
ATOM	2357	OD1	ASN	1727	37.188	-13.539	10.781	1.00	46.57
ATOM	2358	ND2	ASN	1727	37.010	-15.536	11.778	1.00	48.30
ATOM	2361	C	ASN	1727	32.958	-14.159	9.786	1.00	38.22
ATOM	2362	O	ASN	1727	32.883	-13.431	8.793	1.00	39.53
ATOM	2363	N	GLU	1728	32.041	-15.076	10.093	1.00	37.33
ATOM	2365	CA	GLU	1728	30.854	-15.312	9.273	1.00	34.24
ATOM	2366	CB	GLU	1728	30.109	-16.551	9.765	1.00	32.82
ATOM	2367	CG	GLU	1728	28.973	-17.000	8.855	1.00	35.84
ATOM	2368	CD	GLU	1728	28.329	-18.306	9.297	1.00	42.16
ATOM	2369	OE1	GLU	1728	28.409	-18.633	10.504	1.00	46.78
ATOM	2370	OE2	GLU	1728	27.734	-18.996	8.440	1.00	38.81
ATOM	2371	C	GLU	1728	29.925	-14.104	9.313	1.00	33.05
ATOM	2372	O	GLU	1728	29.521	-13.574	8.272	1.00	29.58
ATOM	2373	N	LEU	1729	29.608	-13.671	10.527	1.00	32.09
ATOM	2375	CA	LEU	1729	28.741	-12.530	10.710	1.00	32.45
ATOM	2376	CB	LEU	1729	28.351	-12.389	12.170	1.00	32.64
ATOM	2377	CG	LEU	1729	27.311	-13.431	12.575	1.00	34.65
ATOM	2378	CD1	LEU	1729	27.131	-13.388	14.089	1.00	37.18
ATOM	2379	CD2	LEU	1729	25.988	-13.167	11.842	1.00	27.77
ATOM	2380	C	LEU	1729	29.359	-11.252	10.175	1.00	32.68
ATOM	2381	O	LEU	1729	28.638	-10.367	9.693	1.00	31.97
ATOM	2382	N	TYR	1730	30.688	-11.143	10.251	1.00	31.70
ATOM	2384	CA	TYR	1730	31.378	-9.959	9.734	1.00	30.19
ATOM	2385	CB	TYR	1730	32.849	-9.940	10.154	1.00	27.88
ATOM	2386	CG	TYR	1730	33.591	-8.723	9.649	1.00	26.63
ATOM	2387	CD1	TYR	1730	33.093	-7.449	9.879	1.00	27.37
ATOM	2388	CE1	TYR	1730	33.725	-6.324	9.378	1.00	27.56
ATOM	2389	CD2	TYR	1730	34.759	-8.849	8.904	1.00	24.07
ATOM	2390	CE2	TYR	1730	35.408	-7.724	8.393	1.00	24.81
ATOM	2391	CZ	TYR	1730	34.882	-6.462	8.631	1.00	28.56
ATOM	2392	OH	TYR	1730	35.473	-5.316	8.111	1.00	29.08
ATOM	2394	C	TYR	1730	31.287	-9.962	8.208	1.00	29.50
ATOM	2395	O	TYR	1730	31.062	-8.928	7.585	1.00	29.16
ATOM	2396	N	MET	1731	31.443	-11.139	7.623	1.00	31.05
ATOM	2398	CA	MET	1731	31.366	-11.313	6.187	1.00	34.59
ATOM	2399	CB	MET	1731	31.611	-12.779	5.840	1.00	41.42
ATOM	2400	CG	MET	1731	31.315	-13.149	4.403	1.00	52.20
ATOM	2401	SD	MET	1731	31.801	-14.840	3.994	1.00	64.38
ATOM	2402	CE	MET	1731	32.926	-14.502	2.606	1.00	63.03
ATOM	2403	C	MET	1731	29.992	-10.869	5.695	1.00	34.53
ATOM	2404	O	MET	1731	29.863	-10.268	4.619	1.00	35.08
ATOM	2405	N	MET	1732	28.971	-11.153	6.501	1.00	33.32

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ATOM	2407	CA	MET	1732	27.594	-10.770	6.194	1.00	31.78
ATOM	2408	CB	MET	1732	26.634	-11.346	7.236	1.00	30.42
ATOM	2409	CG	MET	1732	25.172	-11.071	6.938	1.00	30.28
ATOM	2410	SD	MET	1732	24.071	-11.709	8.183	1.00	27.41
ATOM	2411	CE	MET	1732	23.738	-13.369	7.471	1.00	22.35
ATOM	2412	C	MET	1732	27.484	-9.243	6.158	1.00	31.10
ATOM	2413	O	MET	1732	26.794	-8.680	5.303	1.00	31.08
ATOM	2414	N	MET	1733	28.139	-8.586	7.114	1.00	31.22
ATOM	2416	CA	MET	1733	28.161	-7.128	7.189	1.00	30.93
ATOM	2417	CB	MET	1733	29.001	-6.665	8.376	1.00	31.91
ATOM	2418	CG	MET	1733	28.368	-6.906	9.710	1.00	33.63
ATOM	2419	SD	MET	1733	29.375	-6.210	11.021	1.00	34.53
ATOM	2420	CE	MET	1733	29.106	-7.395	12.280	1.00	34.12
ATOM	2421	C	MET	1733	28.830	-6.623	5.921	1.00	32.49
ATOM	2422	O	MET	1733	28.357	-5.682	5.281	1.00	33.61
ATOM	2423	N	ARG	1734	29.932	-7.269	5.551	1.00	32.11
ATOM	2425	CA	ARG	1734	30.673	-6.889	4.355	1.00	31.13
ATOM	2426	CB	ARG	1734	32.012	-7.623	4.308	1.00	28.68
ATOM	2427	CG	ARG	1734	32.953	-7.267	5.451	1.00	27.19
ATOM	2428	CD	ARG	1734	33.159	-5.766	5.558	1.00	26.80
ATOM	2429	NE	ARG	1734	33.864	-5.243	4.393	1.00	35.67
ATOM	2431	CZ	ARG	1734	35.187	-5.305	4.223	1.00	38.03
ATOM	2432	NH1	ARG	1734	35.967	-5.861	5.148	1.00	38.07
ATOM	2435	NH2	ARG	1734	35.729	-4.850	3.094	1.00	38.87
ATOM	2438	C	ARG	1734	29.873	-7.098	3.065	1.00	29.53
ATOM	2439	O	ARG	1734	30.029	-6.334	2.121	1.00	29.11
ATOM	2440	N	ASP	1735	29.036	-8.137	3.025	1.00	29.48
ATOM	2442	CA	ASP	1735	28.193	-8.412	1.859	1.00	26.82
ATOM	2443	CB	ASP	1735	27.591	-9.811	1.933	1.00	30.25
ATOM	2444	CG	ASP	1735	28.632	-10.895	1.773	1.00	35.13
ATOM	2445	OD1	ASP	1735	29.626	-10.645	1.052	1.00	35.19
ATOM	2446	OD2	ASP	1735	28.458	-11.990	2.366	1.00	39.35
ATOM	2447	C	ASP	1735	27.082	-7.375	1.760	1.00	23.88
ATOM	2448	O	ASP	1735	26.692	-6.992	0.656	1.00	24.83
ATOM	2449	N	CYS	1736	26.574	-6.929	2.913	1.00	22.13
ATOM	2451	CA	CYS	1736	25.538	-5.887	2.965	1.00	21.74
ATOM	2452	CB	CYS	1736	25.005	-5.692	4.401	1.00	20.46
ATOM	2453	SG	CYS	1736	23.978	-7.013	5.053	1.00	19.59
ATOM	2454	C	CYS	1736	26.104	-4.542	2.456	1.00	20.51
ATOM	2455	O	CYS	1736	25.377	-3.732	1.887	1.00	16.07
ATOM	2456	N	TRP	1737	27.401	-4.325	2.670	1.00	21.58
ATOM	2458	CA	TRP	1737	28.080	-3.113	2.248	1.00	20.57
ATOM	2459	CB	TRP	1737	29.107	-2.682	3.291	1.00	17.02
ATOM	2460	CG	TRP	1737	28.558	-2.415	4.654	1.00	20.35
ATOM	2461	CD2	TRP	1737	29.254	-2.564	5.897	1.00	20.42
ATOM	2462	CE2	TRP	1737	28.387	-2.122	6.923	1.00	21.18
ATOM	2463	CE3	TRP	1737	30.538	-3.027	6.243	1.00	21.60
ATOM	2464	CD1	TRP	1737	27.317	-1.914	4.970	1.00	19.86
ATOM	2465	NE1	TRP	1737	27.210	-1.732	6.328	1.00	21.03
ATOM	2467	CZ2	TRP	1737	28.760	-2.125	8.276	1.00	21.70
ATOM	2468	CZ3	TRP	1737	30.910	-3.031	7.594	1.00	21.73
ATOM	2469	CH2	TRP	1737	30.025	-2.584	8.588	1.00	23.06

ATOM	2470	C	TRP	1737	28.770	-3.281	0.899	1.00	24.98
ATOM	2471	O	TRP	1737	29.758	-2.607	0.610	1.00	25.84
ATOM	2472	N	HIS	1738	28.269	-4.185	0.063	1.00	27.61
ATOM	2474	CA	HIS	1738	28.885	-4.352	-1.243	1.00	25.81
ATOM	2475	CB	HIS	1738	28.263	-5.522	-2.013	1.00	24.74
ATOM	2476	CG	HIS	1738	29.105	-6.005	-3.162	1.00	26.07
ATOM	2477	CD2	HIS	1738	29.599	-5.353	-4.246	1.00	25.45
ATOM	2478	ND1	HIS	1738	29.571	-7.299	-3.252	1.00	24.60
ATOM	2480	CE1	HIS	1738	30.320	-7.422	-4.333	1.00	24.62
ATOM	2481	NE2	HIS	1738	30.352	-6.253	-4.954	1.00	23.97
ATOM	2483	C	HIS	1738	28.734	-3.034	-2.017	1.00	26.41
ATOM	2484	O	HIS	1738	27.705	-2.350	-1.931	1.00	25.20
ATOM	2485	N	ALA	1739	29.792	-2.658	-2.727	1.00	26.45
ATOM	2487	CA	ALA	1739	29.829	-1.437	-3.517	1.00	25.61
ATOM	2488	CB	ALA	1739	31.193	-1.285	-4.117	1.00	25.87
ATOM	2489	C	ALA	1739	28.765	-1.418	-4.617	1.00	26.67
ATOM	2490	O	ALA	1739	28.207	-0.367	-4.930	1.00	28.28
ATOM	2491	N	VAL	1740	28.529	-2.573	-5.235	1.00	25.10
ATOM	2493	CA	VAL	1740	27.526	-2.706	-6.292	1.00	24.14
ATOM	2494	CB	VAL	1740	27.969	-3.737	-7.378	1.00	24.27
ATOM	2495	CG1	VAL	1740	26.979	-3.792	-8.503	1.00	20.03
ATOM	2496	CG2	VAL	1740	29.331	-3.375	-7.926	1.00	26.74
ATOM	2497	C	VAL	1740	26.234	-3.196	-5.639	1.00	23.91
ATOM	2498	O	VAL	1740	26.173	-4.349	-5.175	1.00	26.37
ATOM	2499	N	PRO	1741	25.173	-2.357	-5.653	1.00	24.55
ATOM	2500	CD	PRO	1741	25.096	-1.065	-6.369	1.00	17.73
ATOM	2501	CA	PRO	1741	23.868	-2.686	-5.058	1.00	22.27
ATOM	2502	CB	PRO	1741	22.979	-1.536	-5.545	1.00	17.82
ATOM	2503	CG	PRO	1741	23.925	-0.410	-5.710	1.00	13.27
ATOM	2504	C	PRO	1741	23.275	-4.057	-5.418	1.00	24.04
ATOM	2505	O	PRO	1741	22.735	-4.748	-4.548	1.00	25.86
ATOM	2506	N	SER	1742	23.431	-4.471	-6.674	1.00	24.30
ATOM	2508	CA	SER	1742	22.888	-5.745	-7.167	1.00	24.42
ATOM	2509	CB	SER	1742	22.986	-5.819	-8.696	1.00	23.95
ATOM	2510	OG	SER	1742	24.334	-5.784	-9.131	1.00	22.98
ATOM	2512	C	SER	1742	23.553	-6.978	-6.589	1.00	25.20
ATOM	2513	O	SER	1742	22.994	-8.085	-6.677	1.00	23.68
ATOM	2514	N	GLN	1743	24.753	-6.793	-6.037	1.00	25.46
ATOM	2516	CA	GLN	1743	25.504	-7.910	-5.485	1.00	25.64
ATOM	2517	CB	GLN	1743	26.993	-7.773	-5.807	1.00	24.02
ATOM	2518	CG	GLN	1743	27.263	-7.768	-7.295	1.00	22.75
ATOM	2519	CD	GLN	1743	26.585	-8.938	-8.014	1.00	26.21
ATOM	2520	OE1	GLN	1743	26.999	-10.087	-7.864	1.00	28.67
ATOM	2521	NE2	GLN	1743	25.535	-8.649	-8.787	1.00	21.57
ATOM	2524	C	GLN	1743	25.270	-8.148	-4.007	1.00	24.86
ATOM	2525	O	GLN	1743	25.685	-9.173	-3.456	1.00	25.24
ATOM	2526	N	ARG	1744	24.525	-7.244	-3.389	1.00	23.38
ATOM	2528	CA	ARG	1744	24.230	-7.376	-1.976	1.00	22.41
ATOM	2529	CB	ARG	1744	23.727	-6.055	-1.415	1.00	22.24
ATOM	2530	CG	ARG	1744	24.718	-4.909	-1.523	1.00	22.53
ATOM	2531	CD	ARG	1744	24.084	-3.577	-1.134	1.00	19.82
ATOM	2532	NE	ARG	1744	24.963	-2.475	-1.517	1.00	22.51

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ATOM	2534	CZ	ARG	1744	24.592	-1.201	-1.663	1.00	22.92
ATOM	2535	NH1	ARG	1744	23.332	-0.814	-1.458	1.00	18.28
ATOM	2538	NH2	ARG	1744	25.491	-0.310	-2.060	1.00	22.15
ATOM	2541	C	ARG	1744	23.163	-8.458	-1.833	1.00	24.61
ATOM	2542	O	ARG	1744	22.428	-8.755	-2.786	1.00	26.94
ATOM	2543	N	PRO	1745	23.143	-9.155	-0.688	1.00	23.21
ATOM	2544	CD	PRO	1745	24.052	-9.107	0.470	1.00	22.38
ATOM	2545	CA	PRO	1745	22.129	-10.190	-0.522	1.00	22.24
ATOM	2546	CB	PRO	1745	22.623	-10.942	0.711	1.00	21.13
ATOM	2547	CG	PRO	1745	23.286	-9.864	1.504	1.00	20.24
ATOM	2548	C	PRO	1745	20.800	-9.506	-0.256	1.00	23.11
ATOM	2549	O	PRO	1745	20.743	-8.300	0.020	1.00	25.93
ATOM	2550	N	THR	1746	19.724	-10.256	-0.373	1.00	20.82
ATOM	2552	CA	THR	1746	18.420	-9.697	-0.112	1.00	20.47
ATOM	2553	CB	THR	1746	17.386	-10.342	-1.041	1.00	18.61
ATOM	2554	OG1	THR	1746	17.382	-11.755	-0.822	1.00	21.86
ATOM	2556	CG2	THR	1746	17.746	-10.078	-2.487	1.00	21.13
ATOM	2557	C	THR	1746	18.060	-9.970	1.344	1.00	20.84
ATOM	2558	O	THR	1746	18.787	-10.674	2.055	1.00	22.08
ATOM	2559	N	PHE	1747	16.953	-9.406	1.810	1.00	21.58
ATOM	2561	CA	PHE	1747	16.536	-9.675	3.178	1.00	21.15
ATOM	2562	CB	PHE	1747	15.442	-8.710	3.613	1.00	20.34
ATOM	2563	CG	PHE	1747	15.961	-7.350	3.982	1.00	23.18
ATOM	2564	CD1	PHE	1747	16.729	-7.170	5.130	1.00	22.26
ATOM	2565	CD2	PHE	1747	15.668	-6.240	3.196	1.00	23.41
ATOM	2566	CE1	PHE	1747	17.186	-5.909	5.484	1.00	17.31
ATOM	2567	CE2	PHE	1747	16.124	-4.967	3.548	1.00	17.93
ATOM	2568	CZ	PHE	1747	16.883	-4.809	4.696	1.00	19.06
ATOM	2569	C	PHE	1747	16.062	-11.124	3.217	1.00	21.61
ATOM	2570	O	PHE	1747	16.248	-11.823	4.212	1.00	22.19
ATOM	2571	N	LYS	1748	15.490	-11.588	2.111	1.00	22.00
ATOM	2573	CA	LYS	1748	15.048	-12.973	2.009	1.00	24.34
ATOM	2574	CB	LYS	1748	14.471	-13.227	0.621	1.00	23.61
ATOM	2575	CG	LYS	1748	14.050	-14.663	0.416	1.00	27.45
ATOM	2576	CD	LYS	1748	13.633	-14.932	-0.998	1.00	28.97
ATOM	2577	CE	LYS	1748	13.244	-16.394	-1.163	1.00	35.95
ATOM	2578	NZ	LYS	1748	12.213	-16.795	-0.153	1.00	41.69
ATOM	2582	C	LYS	1748	16.257	-13.907	2.264	1.00	27.58
ATOM	2583	O	LYS	1748	16.161	-14.863	3.034	1.00	29.73
ATOM	2584	N	GLN	1749	17.397	-13.604	1.640	1.00	25.88
ATOM	2586	CA	GLN	1749	18.617	-14.394	1.804	1.00	23.72
ATOM	2587	CB	GLN	1749	19.692	-13.925	0.837	1.00	27.00
ATOM	2588	CG	GLN	1749	19.338	-13.954	-0.628	1.00	32.28
ATOM	2589	CD	GLN	1749	20.442	-13.331	-1.477	1.00	36.35
ATOM	2590	OE1	GLN	1749	20.175	-12.528	-2.368	1.00	37.63
ATOM	2591	NE2	GLN	1749	21.699	-13.702	-1.194	1.00	38.60
ATOM	2594	C	GLN	1749	19.177	-14.266	3.212	1.00	23.44
ATOM	2595	O	GLN	1749	19.586	-15.260	3.826	1.00	23.52
ATOM	2596	N	LEU	1750	19.267	-13.035	3.703	1.00	21.73
ATOM	2598	CA	LEU	1750	19.787	-12.796	5.054	1.00	20.90
ATOM	2599	CB	LEU	1750	19.752	-11.308	5.359	1.00	18.60
ATOM	2600	CG	LEU	1750	20.654	-10.439	4.485	1.00	16.53

ATOM	2601	CD1	LEU	1750	20.190	-8.979	4.579	1.00	13.28
ATOM	2602	CD2	LEU	1750	22.100	-10.612	4.939	1.00	14.74
ATOM	2603	C	LEU	1750	18.982	-13.548	6.108	1.00	21.25
ATOM	2604	O	LEU	1750	19.534	-14.056	7.084	1.00	21.26
ATOM	2605	N	VAL	1751	17.671	-13.607	5.917	1.00	21.64
ATOM	2607	CA	VAL	1751	16.793	-14.289	6.845	1.00	21.21
ATOM	2608	CB	VAL	1751	15.353	-14.072	6.432	1.00	19.03
ATOM	2609	CG1	VAL	1751	14.453	-14.970	7.220	1.00	23.34
ATOM	2610	CG2	VAL	1751	14.978	-12.648	6.684	1.00	22.78
ATOM	2611	C	VAL	1751	17.127	-15.774	6.925	1.00	25.56
ATOM	2612	O	VAL	1751	17.111	-16.369	8.007	1.00	25.61
ATOM	2613	N	GLU	1752	17.418	-16.381	5.778	1.00	28.61
ATOM	2615	CA	GLU	1752	17.773	-17.789	5.755	1.00	32.38
ATOM	2616	CB	GLU	1752	17.765	-18.317	4.321	1.00	37.26
ATOM	2617	CG	GLU	1752	16.399	-18.218	3.651	1.00	44.76
ATOM	2618	CD	GLU	1752	16.394	-18.742	2.219	1.00	50.37
ATOM	2619	OE1	GLU	1752	15.397	-18.495	1.497	1.00	52.52
ATOM	2620	OE2	GLU	1752	17.377	-19.410	1.822	1.00	51.96
ATOM	2621	C	GLU	1752	19.140	-17.984	6.405	1.00	32.27
ATOM	2622	O	GLU	1752	19.330	-18.878	7.237	1.00	31.18
ATOM	2623	N	ASP	1753	20.069	-17.096	6.083	1.00	33.20
ATOM	2625	CA	ASP	1753	21.411	-17.174	6.647	1.00	35.13
ATOM	2626	CB	ASP	1753	22.341	-16.144	5.998	1.00	37.80
ATOM	2627	CG	ASP	1753	22.498	-16.358	4.502	1.00	41.13
ATOM	2628	OD1	ASP	1753	22.222	-17.470	4.007	1.00	43.01
ATOM	2629	OD2	ASP	1753	22.908	-15.401	3.811	1.00	44.26
ATOM	2630	C	ASP	1753	21.378	-16.986	8.163	1.00	33.84
ATOM	2631	O	ASP	1753	21.971	-17.773	8.901	1.00	36.22
ATOM	2632	N	LEU	1754	20.652	-15.978	8.633	1.00	30.73
ATOM	2634	CA	LEU	1754	20.568	-15.730	10.070	1.00	28.51
ATOM	2635	CB	LEU	1754	19.881	-14.394	10.355	1.00	25.20
ATOM	2636	CG	LEU	1754	20.810	-13.225	10.016	1.00	26.72
ATOM	2637	CD1	LEU	1754	20.045	-11.903	9.905	1.00	24.18
ATOM	2638	CD2	LEU	1754	21.932	-13.168	11.063	1.00	25.69
ATOM	2639	C	LEU	1754	19.860	-16.870	10.763	1.00	28.74
ATOM	2640	O	LEU	1754	20.270	-17.290	11.832	1.00	29.08
ATOM	2641	N	ASP	1755	18.834	-17.419	10.130	1.00	29.97
ATOM	2643	CA	ASP	1755	18.109	-18.519	10.732	1.00	31.58
ATOM	2644	CB	ASP	1755	16.944	-18.930	9.843	1.00	36.47
ATOM	2645	CG	ASP	1755	16.100	-20.005	10.467	1.00	39.40
ATOM	2646	OD1	ASP	1755	15.731	-19.869	11.651	1.00	45.91
ATOM	2647	OD2	ASP	1755	15.813	-20.995	9.774	1.00	45.68
ATOM	2648	C	ASP	1755	19.040	-19.703	10.952	1.00	32.29
ATOM	2649	O	ASP	1755	18.978	-20.380	11.979	1.00	31.66
ATOM	2650	N	ARG	1756	19.926	-19.923	9.989	1.00	32.32
ATOM	2652	CA	ARG	1756	20.884	-21.015	10.059	1.00	32.73
ATOM	2653	CB	ARG	1756	21.598	-21.145	8.704	1.00	34.47
ATOM	2654	CG	ARG	1756	22.733	-22.157	8.645	1.00	37.78
ATOM	2655	CD	ARG	1756	23.299	-22.274	7.237	1.00	43.87
ATOM	2656	NE	ARG	1756	23.791	-20.999	6.702	1.00	48.78
ATOM	2658	CZ	ARG	1756	24.890	-20.380	7.122	1.00	52.92
ATOM	2659	NH1	ARG	1756	25.630	-20.914	8.091	1.00	55.88

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ATOM	2662	NH2	ARG	1756	25.237	-19.214	6.593	1.00	52.53
ATOM	2665	C	ARG	1756	21.889	-20.761	11.186	1.00	33.76
ATOM	2666	O	ARG	1756	22.131	-21.619	12.049	1.00	34.53
ATOM	2667	N	ILE	1757	22.432	-19.553	11.204	1.00	33.49
ATOM	2669	CA	ILE	1757	23.405	-19.176	12.205	1.00	32.71
ATOM	2670	CB	ILE	1757	23.980	-17.764	11.919	1.00	31.86
ATOM	2671	CG2	ILE	1757	25.111	-17.454	12.869	1.00	31.71
ATOM	2672	CG1	ILE	1757	24.520	-17.704	10.488	1.00	31.41
ATOM	2673	CD1	ILE	1757	25.075	-16.366	10.096	1.00	27.68
ATOM	2674	C	ILE	1757	22.807	-19.236	13.604	1.00	34.20
ATOM	2675	O	ILE	1757	23.399	-19.833	14.495	1.00	35.83
ATOM	2676	N	VAL	1758	21.620	-18.667	13.792	1.00	35.40
ATOM	2678	CA	VAL	1758	20.981	-18.653	15.108	1.00	37.49
ATOM	2679	CB	VAL	1758	19.501	-18.160	15.061	1.00	34.42
ATOM	2680	CG1	VAL	1758	18.899	-18.199	16.456	1.00	37.37
ATOM	2681	CG2	VAL	1758	19.403	-16.742	14.519	1.00	30.02
ATOM	2682	C	VAL	1758	21.010	-20.050	15.715	1.00	41.64
ATOM	2683	O	VAL	1758	21.533	-20.246	16.817	1.00	43.69
ATOM	2684	N	ALA	1759	20.492	-21.015	14.961	1.00	44.52
ATOM	2686	CA	ALA	1759	20.434	-22.415	15.387	1.00	45.20
ATOM	2687	CB	ALA	1759	19.833	-23.268	14.277	1.00	43.44
ATOM	2688	C	ALA	1759	21.791	-22.968	15.795	1.00	45.91
ATOM	2689	O	ALA	1759	21.890	-23.780	16.710	1.00	47.41
ATOM	2690	N	LEU	1760	22.833	-22.511	15.120	1.00	47.70
ATOM	2692	CA	LEU	1760	24.190	-22.960	15.399	1.00	50.91
ATOM	2693	CB	LEU	1760	25.015	-22.912	14.109	1.00	52.93
ATOM	2694	CG	LEU	1760	24.448	-23.723	12.947	1.00	57.55
ATOM	2695	CD1	LEU	1760	25.189	-23.390	11.660	1.00	60.76
ATOM	2696	CD2	LEU	1760	24.539	-25.208	13.273	1.00	58.66
ATOM	2697	C	LEU	1760	24.882	-22.111	16.472	1.00	52.07
ATOM	2698	O	LEU	1760	25.967	-22.459	16.953	1.00	51.95
ATOM	2699	N	THR	1761	24.267	-21.000	16.850	1.00	52.05
ATOM	2701	CA	THR	1761	24.868	-20.131	17.836	1.00	53.28
ATOM	2702	CB	THR	1761	24.362	-18.693	17.673	1.00	54.58
ATOM	2703	OG1	THR	1761	24.633	-18.259	16.339	1.00	53.68
ATOM	2705	CG2	THR	1761	25.090	-17.762	18.621	1.00	55.45
ATOM	2706	C	THR	1761	24.715	-20.619	19.272	1.00	53.31
ATOM	2707	O	THR	1761	23.629	-20.986	19.713	1.00	53.89
ATOM	2708	N	SER	1762	25.832	-20.617	19.993	1.00	53.51
ATOM	2710	CA	SER	1762	25.876	-21.045	21.383	1.00	53.15
ATOM	2711	CB	SER	1762	27.340	-21.131	21.830	1.00	57.27
ATOM	2712	OG	SER	1762	27.492	-21.872	23.028	1.00	61.22
ATOM	2714	C	SER	1762	25.110	-20.048	22.257	1.00	49.15
ATOM	2715	O	SER	1762	25.229	-18.831	22.071	1.00	46.61
ATOM	3466	N	ALA	461	79.636	26.047	14.493	1.00	61.05
ATOM	3468	CA	ALA	461	79.609	24.852	13.654	1.00	58.10
ATOM	3469	CB	ALA	461	78.335	24.024	13.935	1.00	60.39
ATOM	3470	C	ALA	461	79.694	25.239	12.179	1.00	54.65
ATOM	3471	O	ALA	461	79.653	24.382	11.297	1.00	54.05
ATOM	3472	N	ALA	462	79.867	26.537	11.935	1.00	51.68
ATOM	3474	CA	ALA	462	79.972	27.085	10.584	1.00	48.47
ATOM	3475	CB	ALA	462	80.099	28.619	10.633	1.00	46.99

ATOM	3476	C	ALA	462	81.123	26.489	9.766	1.00	44.86
ATOM	3477	O	ALA	462	80.918	26.097	8.625	1.00	43.40
ATOM	3478	N	TYR	463	82.329	26.447	10.335	1.00	42.23
ATOM	3480	CA	TYR	463	83.493	25.913	9.629	1.00	39.04
ATOM	3481	CB	TYR	463	84.642	26.921	9.620	1.00	39.01
ATOM	3482	CG	TYR	463	84.354	28.126	8.743	1.00	41.95
ATOM	3483	CD1	TYR	463	84.073	29.373	9.308	1.00	42.40
ATOM	3484	CE1	TYR	463	83.754	30.466	8.512	1.00	42.02
ATOM	3485	CD2	TYR	463	84.311	28.009	7.345	1.00	40.70
ATOM	3486	CE2	TYR	463	83.992	29.099	6.542	1.00	37.09
ATOM	3487	CZ	TYR	463	83.716	30.320	7.134	1.00	39.19
ATOM	3488	OH	TYR	463	83.401	31.406	6.360	1.00	40.66
ATOM	3490	C	TYR	463	84.011	24.554	10.050	1.00	37.78
ATOM	3491	O	TYR	463	84.627	23.863	9.237	1.00	38.35
ATOM	3492	N	GLU	464	83.746	24.143	11.285	1.00	37.67
ATOM	3494	CA	GLU	464	84.212	22.841	11.747	1.00	38.57
ATOM	3495	CB	GLU	464	85.707	22.890	12.024	1.00	41.44
ATOM	3496	CG	GLU	464	86.093	23.870	13.108	1.00	47.87
ATOM	3497	CD	GLU	464	87.583	24.135	13.169	1.00	53.44
ATOM	3498	OE1	GLU	464	87.998	24.983	13.990	1.00	56.72
ATOM	3499	OE2	GLU	464	88.344	23.513	12.397	1.00	54.85
ATOM	3500	C	GLU	464	83.504	22.393	13.001	1.00	38.15
ATOM	3501	O	GLU	464	83.291	23.187	13.905	1.00	39.59
ATOM	3502	N	LEU	465	83.121	21.124	13.051	1.00	37.13
ATOM	3504	CA	LEU	465	82.457	20.608	14.236	1.00	37.93
ATOM	3505	CB	LEU	465	81.502	19.456	13.894	1.00	33.43
ATOM	3506	CG	LEU	465	80.455	19.609	12.787	1.00	31.12
ATOM	3507	CD1	LEU	465	79.415	18.500	12.944	1.00	24.85
ATOM	3508	CD2	LEU	465	79.797	20.980	12.855	1.00	29.05
ATOM	3509	C	LEU	465	83.540	20.090	15.166	1.00	41.02
ATOM	3510	O	LEU	465	84.703	19.936	14.763	1.00	40.24
ATOM	3511	N	PRO	466	83.198	19.884	16.441	1.00	43.58
ATOM	3512	CD	PRO	466	81.974	20.359	17.115	1.00	45.33
ATOM	3513	CA	PRO	466	84.170	19.374	17.415	1.00	44.72
ATOM	3514	CB	PRO	466	83.433	19.505	18.743	1.00	46.18
ATOM	3515	CG	PRO	466	82.486	20.679	18.496	1.00	48.84
ATOM	3516	C	PRO	466	84.447	17.909	17.101	1.00	44.52
ATOM	3517	O	PRO	466	83.616	17.228	16.509	1.00	43.38
ATOM	3518	N	GLU	467	85.610	17.421	17.492	1.00	47.75
ATOM	3520	CA	GLU	467	85.932	16.035	17.218	1.00	51.03
ATOM	3521	CB	GLU	467	87.354	15.913	16.659	1.00	56.11
ATOM	3522	CG	GLU	467	87.615	14.557	16.000	1.00	62.27
ATOM	3523	CD	GLU	467	88.927	14.489	15.242	1.00	66.39
ATOM	3524	OE1	GLU	467	89.688	15.490	15.243	1.00	69.85
ATOM	3525	OE2	GLU	467	89.182	13.418	14.643	1.00	66.09
ATOM	3526	C	GLU	467	85.749	15.136	18.435	1.00	49.62
ATOM	3527	O	GLU	467	85.767	15.601	19.578	1.00	49.62
ATOM	3528	N	ASP	468	85.516	13.856	18.166	1.00	48.07
ATOM	3530	CA	ASP	468	85.352	12.843	19.198	1.00	46.32
ATOM	3531	CB	ASP	468	83.880	12.679	19.587	1.00	45.15
ATOM	3532	CG	ASP	468	83.678	11.740	20.779	1.00	44.19
ATOM	3533	OD1	ASP	468	82.544	11.709	21.309	1.00	42.04

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ATOM	3534	OD2	ASP	468	84.629	11.033	21.188	1.00	38.14
ATOM	3535	C	ASP	468	85.877	11.556	18.580	1.00	45.54
ATOM	3536	O	ASP	468	85.141	10.815	17.928	1.00	45.94
ATOM	3537	N	PRO	469	87.181	11.308	18.732	1.00	45.89
ATOM	3538	CD	PRO	469	88.111	12.189	19.464	1.00	45.11
ATOM	3539	CA	PRO	469	87.885	10.130	18.215	1.00	45.91
ATOM	3540	CB	PRO	469	89.208	10.187	18.968	1.00	45.90
ATOM	3541	CG	PRO	469	89.456	11.662	19.042	1.00	45.73
ATOM	3542	C	PRO	469	87.170	8.806	18.473	1.00	45.48
ATOM	3543	O	PRO	469	87.188	7.905	17.629	1.00	46.83
ATOM	3544	N	ARG	470	86.495	8.717	19.613	1.00	42.12
ATOM	3546	CA	ARG	470	85.786	7.506	19.999	1.00	41.21
ATOM	3547	CB	ARG	470	85.083	7.704	21.331	1.00	43.14
ATOM	3548	CG	ARG	470	85.885	8.424	22.375	1.00	45.68
ATOM	3549	CD	ARG	470	85.014	8.705	23.564	1.00	45.98
ATOM	3550	NE	ARG	470	83.802	9.417	23.184	1.00	47.28
ATOM	3552	CZ	ARG	470	82.921	9.877	24.057	1.00	50.54
ATOM	3553	NH1	ARG	470	83.127	9.687	25.354	1.00	47.56
ATOM	3556	NH2	ARG	470	81.843	10.527	23.637	1.00	54.59
ATOM	3559	C	ARG	470	84.736	7.058	19.004	1.00	40.57
ATOM	3560	O	ARG	470	84.411	5.877	18.941	1.00	43.13
ATOM	3561	N	TRP	471	84.182	8.014	18.268	1.00	38.07
ATOM	3563	CA	TRP	471	83.124	7.736	17.314	1.00	35.09
ATOM	3564	CB	TRP	471	81.890	8.515	17.739	1.00	33.42
ATOM	3565	CG	TRP	471	81.259	7.958	18.952	1.00	31.71
ATOM	3566	CD2	TRP	471	80.512	6.740	19.026	1.00	34.81
ATOM	3567	CE2	TRP	471	80.061	6.610	20.355	1.00	33.17
ATOM	3568	CE3	TRP	471	80.174	5.744	18.092	1.00	37.60
ATOM	3569	CD1	TRP	471	81.246	8.503	20.199	1.00	25.70
ATOM	3570	NE1	TRP	471	80.525	7.697	21.051	1.00	28.79
ATOM	3572	CZ2	TRP	471	79.289	5.522	20.776	1.00	35.80
ATOM	3573	CZ3	TRP	471	79.409	4.660	18.509	1.00	35.52
ATOM	3574	CH2	TRP	471	78.973	4.560	19.839	1.00	34.51
ATOM	3575	C	TRP	471	83.432	8.065	15.872	1.00	35.77
ATOM	3576	O	TRP	471	82.690	7.670	14.968	1.00	37.45
ATOM	3577	N	GLU	472	84.533	8.770	15.651	1.00	34.76
ATOM	3579	CA	GLU	472	84.895	9.184	14.308	1.00	34.51
ATOM	3580	CB	GLU	472	86.065	10.174	14.365	1.00	32.30
ATOM	3581	CG	GLU	472	86.221	11.038	13.103	1.00	36.57
ATOM	3582	CD	GLU	472	85.082	12.035	12.872	1.00	36.34
ATOM	3583	OE1	GLU	472	84.515	12.558	13.857	1.00	36.01
ATOM	3584	OE2	GLU	472	84.777	12.318	11.694	1.00	31.95
ATOM	3585	C	GLU	472	85.219	8.034	13.364	1.00	33.90
ATOM	3586	O	GLU	472	85.896	7.082	13.745	1.00	33.77
ATOM	3587	N	LEU	473	84.667	8.094	12.158	1.00	33.58
ATOM	3589	CA	LEU	473	84.944	7.095	11.146	1.00	34.82
ATOM	3590	CB	LEU	473	83.714	6.234	10.847	1.00	32.59
ATOM	3591	CG	LEU	473	84.020	5.091	9.867	1.00	33.78
ATOM	3592	CD1	LEU	473	84.786	4.000	10.578	1.00	32.94
ATOM	3593	CD2	LEU	473	82.759	4.518	9.273	1.00	35.34
ATOM	3594	C	LEU	473	85.380	7.828	9.883	1.00	37.95
ATOM	3595	O	LEU	473	84.720	8.781	9.457	1.00	39.55

ATOM	3596	N	PRO	474	86.522	7.423	9.299	1.00	38.99
ATOM	3597	CD	PRO	474	87.455	6.453	9.899	1.00	38.76
ATOM	3598	CA	PRO	474	87.094	8.004	8.080	1.00	39.37
ATOM	3599	CB	PRO	474	88.382	7.201	7.906	1.00	40.18
ATOM	3600	CG	PRO	474	88.767	6.883	9.310	1.00	37.76
ATOM	3601	C	PRO	474	86.165	7.794	6.890	1.00	40.94
ATOM	3602	O	PRO	474	85.865	6.653	6.532	1.00	43.98
ATOM	3603	N	ARG	475	85.762	8.886	6.245	1.00	40.66
ATOM	3605	CA	ARG	475	84.850	8.840	5.101	1.00	40.66
ATOM	3606	CB	ARG	475	84.776	10.216	4.448	1.00	37.94
ATOM	3607	CG	ARG	475	84.354	11.300	5.415	1.00	36.12
ATOM	3608	CD	ARG	475	84.340	12.697	4.800	1.00	35.92
ATOM	3609	NE	ARG	475	83.932	13.677	5.801	1.00	30.14
ATOM	3611	CZ	ARG	475	82.671	13.878	6.170	1.00	28.45
ATOM	3612	NH1	ARG	475	81.688	13.197	5.599	1.00	28.41
ATOM	3615	NH2	ARG	475	82.410	14.666	7.197	1.00	27.85
ATOM	3618	C	ARG	475	85.141	7.766	4.046	1.00	41.44
ATOM	3619	O	ARG	475	84.223	7.189	3.470	1.00	41.40
ATOM	3620	N	ASP	476	86.419	7.475	3.830	1.00	44.99
ATOM	3622	CA	ASP	476	86.836	6.477	2.849	1.00	50.62
ATOM	3623	CB	ASP	476	88.344	6.540	2.644	1.00	54.47
ATOM	3624	CG	ASP	476	89.105	5.969	3.819	1.00	60.03
ATOM	3625	OD1	ASP	476	89.569	4.810	3.722	1.00	65.09
ATOM	3626	OD2	ASP	476	89.216	6.669	4.846	1.00	62.62
ATOM	3627	C	ASP	476	86.436	5.054	3.263	1.00	51.16
ATOM	3628	O	ASP	476	86.678	4.091	2.530	1.00	53.06
ATOM	3629	N	ARG	477	85.900	4.916	4.471	1.00	49.58
ATOM	3631	CA	ARG	477	85.443	3.623	4.968	1.00	47.34
ATOM	3632	CB	ARG	477	86.040	3.359	6.341	1.00	48.85
ATOM	3633	CG	ARG	477	87.481	2.924	6.265	1.00	52.11
ATOM	3634	CD	ARG	477	88.169	3.079	7.591	1.00	53.63
ATOM	3635	NE	ARG	477	87.515	2.345	8.665	1.00	54.86
ATOM	3637	CZ	ARG	477	87.932	2.363	9.927	1.00	57.15
ATOM	3638	NH1	ARG	477	89.000	3.076	10.264	1.00	55.98
ATOM	3641	NH2	ARG	477	87.269	1.691	10.855	1.00	58.31
ATOM	3644	C	ARG	477	83.915	3.563	5.020	1.00	44.70
ATOM	3645	O	ARG	477	83.339	2.780	5.770	1.00	44.63
ATOM	3646	N	LEU	478	83.274	4.366	4.179	1.00	41.95
ATOM	3648	CA	LEU	478	81.832	4.440	4.118	1.00	38.58
ATOM	3649	CB	LEU	478	81.374	5.609	4.980	1.00	33.17
ATOM	3650	CG	LEU	478	79.872	5.731	5.183	1.00	29.07
ATOM	3651	CD1	LEU	478	79.393	4.592	6.052	1.00	28.25
ATOM	3652	CD2	LEU	478	79.590	7.059	5.836	1.00	30.79
ATOM	3653	C	LEU	478	81.432	4.710	2.674	1.00	38.93
ATOM	3654	O	LEU	478	81.938	5.647	2.071	1.00	41.75
ATOM	3655	N	VAL	479	80.562	3.880	2.107	1.00	37.96
ATOM	3657	CA	VAL	479	80.113	4.086	0.730	1.00	37.87
ATOM	3658	CB	VAL	479	80.468	2.882	-0.192	1.00	36.47
ATOM	3659	CG1	VAL	479	80.001	3.145	-1.612	1.00	34.43
ATOM	3660	CG2	VAL	479	81.972	2.651	-0.187	1.00	34.33
ATOM	3661	C	VAL	479	78.609	4.299	0.775	1.00	38.10
ATOM	3662	O	VAL	479	77.846	3.366	1.019	1.00	40.13

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ATOM	3663	N	LEU	480	78.184	5.537	0.552	1.00	38.05
ATOM	3665	CA	LEU	480	76.766	5.879	0.606	1.00	35.90
ATOM	3666	CB	LEU	480	76.568	7.393	0.475	1.00	33.98
ATOM	3667	CG	LEU	480	77.276	8.257	1.536	1.00	32.84
ATOM	3668	CD1	LEU	480	77.003	9.749	1.273	1.00	29.68
ATOM	3669	CD2	LEU	480	76.828	7.861	2.943	1.00	26.03
ATOM	3670	C	LEU	480	76.015	5.146	-0.476	1.00	34.99
ATOM	3671	O	LEU	480	76.573	4.864	-1.526	1.00	36.12
ATOM	3672	N	GLY	481	74.753	4.836	-0.223	1.00	35.21
ATOM	3674	CA	GLY	481	73.965	4.120	-1.204	1.00	34.79
ATOM	3675	C	GLY	481	72.544	4.608	-1.332	1.00	36.31
ATOM	3676	O	GLY	481	72.237	5.775	-1.046	1.00	38.30
ATOM	3677	N	LYS	482	71.665	3.705	-1.761	1.00	35.59
ATOM	3679	CA	LYS	482	70.257	4.007	-1.959	1.00	35.24
ATOM	3680	CB	LYS	482	69.488	2.698	-2.207	1.00	35.69
ATOM	3681	C	LYS	482	69.585	4.763	-0.823	1.00	36.31
ATOM	3682	O	LYS	482	69.752	4.421	0.352	1.00	34.90
ATOM	3683	N	PRO	483	68.787	5.786	-1.157	1.00	38.08
ATOM	3684	CD	PRO	483	68.432	6.320	-2.483	1.00	39.57
ATOM	3685	CA	PRO	483	68.097	6.566	-0.135	1.00	41.08
ATOM	3686	CB	PRO	483	67.300	7.560	-0.987	1.00	39.80
ATOM	3687	CG	PRO	483	68.268	7.819	-2.157	1.00	37.87
ATOM	3688	C	PRO	483	67.130	5.652	0.606	1.00	42.11
ATOM	3689	O	PRO	483	66.306	4.994	-0.025	1.00	43.01
ATOM	3690	N	LEU	484	67.199	5.624	1.937	1.00	41.06
ATOM	3692	CA	LEU	484	66.293	4.823	2.751	1.00	38.47
ATOM	3693	CB	LEU	484	67.040	4.307	3.990	1.00	32.45
ATOM	3694	CG	LEU	484	67.968	3.098	3.809	1.00	27.68
ATOM	3695	CD1	LEU	484	68.569	2.710	5.147	1.00	20.29
ATOM	3696	CD2	LEU	484	67.181	1.964	3.225	1.00	23.20
ATOM	3697	C	LEU	484	65.084	5.637	3.180	1.00	42.18
ATOM	3698	O	LEU	484	65.227	6.699	3.814	1.00	44.50
ATOM	3699	N	GLY	485	63.893	5.170	2.817	1.00	45.68
ATOM	3701	CA	GLY	485	62.692	5.863	3.220	1.00	49.88
ATOM	3702	C	GLY	485	62.216	7.008	2.337	1.00	53.01
ATOM	3703	O	GLY	485	62.438	7.005	1.117	1.00	50.26
ATOM	3704	N	GLU	486	61.592	8.020	2.949	1.00	56.24
ATOM	3706	CA	GLU	486	61.064	9.183	2.257	1.00	58.07
ATOM	3707	CB	GLU	486	59.666	8.845	1.682	1.00	55.60
ATOM	3708	C	GLU	486	60.995	10.477	3.088	1.00	59.35
ATOM	3709	O	GLU	486	60.019	11.226	3.000	1.00	61.44
ATOM	3710	N	GLY	487	62.027	10.747	3.879	1.00	59.60
ATOM	3712	CA	GLY	487	62.066	11.964	4.652	1.00	59.75
ATOM	3713	C	GLY	487	61.337	11.959	5.974	1.00	61.44
ATOM	3714	O	GLY	487	61.231	12.979	6.627	1.00	61.96
ATOM	3715	N	ALA	488	60.820	10.800	6.377	1.00	59.69
ATOM	3717	CA	ALA	488	60.134	10.709	7.657	1.00	57.27
ATOM	3718	CB	ALA	488	59.489	9.337	7.825	1.00	58.05
ATOM	3719	C	ALA	488	61.137	10.970	8.754	1.00	56.28
ATOM	3720	O	ALA	488	60.810	11.446	9.834	1.00	57.31
ATOM	3721	N	PHE	489	62.389	10.630	8.480	1.00	54.40
ATOM	3723	CA	PHE	489	63.462	10.830	9.466	1.00	54.56

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ATOM	3724	CB	PHE	489	64.161	9.500	9.770	1.00	49.88
ATOM	3725	CG	PHE	489	63.222	8.454	10.352	1.00	45.21
ATOM	3726	CD1	PHE	489	62.505	7.585	9.516	1.00	43.48
ATOM	3727	CD2	PHE	489	63.017	8.344	11.738	1.00	40.99
ATOM	3728	CE1	PHE	489	61.625	6.653	10.039	1.00	36.69
ATOM	3729	CE2	PHE	489	62.138	7.411	12.257	1.00	35.02
ATOM	3730	CZ	PHE	489	61.433	6.558	11.407	1.00	34.73
ATOM	3731	C	PHE	489	64.456	11.896	8.974	1.00	56.31
ATOM	3732	O	PHE	489	65.372	12.276	9.692	1.00	59.05
ATOM	3733	N	GLY	490	64.285	12.375	7.735	1.00	56.56
ATOM	3735	CA	GLY	490	65.141	13.400	7.143	1.00	55.60
ATOM	3736	C	GLY	490	65.899	12.778	5.993	1.00	54.79
ATOM	3737	O	GLY	490	65.357	11.854	5.366	1.00	57.10
ATOM	3738	N	GLN	491	67.073	13.304	5.634	1.00	53.44
ATOM	3740	CA	GLN	491	67.829	12.658	4.562	1.00	52.60
ATOM	3741	CB	GLN	491	68.760	13.580	3.777	1.00	53.48
ATOM	3742	CG	GLN	491	69.422	12.818	2.629	1.00	57.19
ATOM	3743	CD	GLN	491	70.046	13.696	1.548	1.00	62.09
ATOM	3744	OE1	GLN	491	70.113	14.893	1.701	1.00	70.26
ATOM	3745	NE2	GLN	491	70.453	13.082	0.441	1.00	62.78
ATOM	3748	C	GLN	491	68.632	11.518	5.165	1.00	49.89
ATOM	3749	O	GLN	491	69.669	11.704	5.805	1.00	49.56
ATOM	3750	N	VAL	492	68.103	10.318	4.984	1.00	47.83
ATOM	3752	CA	VAL	492	68.705	9.093	5.456	1.00	46.38
ATOM	3753	CB	VAL	492	67.760	8.320	6.412	1.00	45.61
ATOM	3754	CG1	VAL	492	68.412	7.045	6.932	1.00	46.70
ATOM	3755	CG2	VAL	492	67.361	9.211	7.606	1.00	46.97
ATOM	3756	C	VAL	492	69.004	8.200	4.253	1.00	45.23
ATOM	3757	O	VAL	492	68.181	8.044	3.349	1.00	45.17
ATOM	3758	N	VAL	493	70.210	7.654	4.208	1.00	43.75
ATOM	3760	CA	VAL	493	70.599	6.780	3.109	1.00	44.71
ATOM	3761	CB	VAL	493	71.608	7.471	2.148	1.00	46.20
ATOM	3762	CG1	VAL	493	71.159	8.902	1.838	1.00	46.16
ATOM	3763	CG2	VAL	493	73.045	7.428	2.706	1.00	42.06
ATOM	3764	C	VAL	493	71.205	5.482	3.624	1.00	44.09
ATOM	3765	O	VAL	493	71.701	5.402	4.745	1.00	43.73
ATOM	3766	N	LEU	494	71.102	4.448	2.809	1.00	43.38
ATOM	3768	CA	LEU	494	71.682	3.158	3.142	1.00	43.29
ATOM	3769	CB	LEU	494	70.988	2.030	2.366	1.00	43.38
ATOM	3770	CG	LEU	494	71.563	0.614	2.431	1.00	39.77
ATOM	3771	CD1	LEU	494	71.809	0.201	3.850	1.00	36.38
ATOM	3772	CD2	LEU	494	70.600	-0.337	1.760	1.00	42.50
ATOM	3773	C	LEU	494	73.139	3.280	2.725	1.00	42.72
ATOM	3774	O	LEU	494	73.435	3.929	1.720	1.00	43.83
ATOM	3775	N	ALA	495	74.044	2.698	3.499	1.00	40.80
ATOM	3777	CA	ALA	495	75.456	2.785	3.183	1.00	43.80
ATOM	3778	CB	ALA	495	76.059	4.032	3.821	1.00	43.76
ATOM	3779	C	ALA	495	76.171	1.546	3.682	1.00	46.68
ATOM	3780	O	ALA	495	75.668	0.838	4.551	1.00	48.52
ATOM	3781	N	GLU	496	77.330	1.258	3.104	1.00	49.13
ATOM	3783	CA	GLU	496	78.112	0.103	3.519	1.00	49.79
ATOM	3784	CB	GLU	496	78.524	-0.732	2.318	1.00	53.83

ATOM	3785	CG	GLU	496	77.350	-1.224	1.496	1.00	61.33
ATOM	3786	CD	GLU	496	77.623	-2.561	0.862	1.00	64.74
ATOM	3787	OE1	GLU	496	76.704	-3.411	0.883	1.00	70.08
ATOM	3788	OE2	GLU	496	78.751	-2.760	0.356	1.00	64.12
ATOM	3789	C	GLU	496	79.333	0.601	4.230	1.00	48.46
ATOM	3790	O	GLU	496	80.192	1.236	3.631	1.00	48.79
ATOM	3791	N	ALA	497	79.373	0.375	5.530	1.00	49.25
ATOM	3793	CA	ALA	497	80.503	0.810	6.334	1.00	49.99
ATOM	3794	CB	ALA	497	80.048	1.156	7.732	1.00	48.16
ATOM	3795	C	ALA	497	81.544	-0.301	6.373	1.00	51.53
ATOM	3796	O	ALA	497	81.191	-1.473	6.409	1.00	52.41
ATOM	3797	N	ILE	498	82.821	0.061	6.335	1.00	52.35
ATOM	3799	CA	ILE	498	83.892	-0.928	6.369	1.00	52.03
ATOM	3800	CB	ILE	498	84.843	-0.797	5.145	1.00	52.83
ATOM	3801	CG2	ILE	498	85.990	-1.795	5.253	1.00	51.43
ATOM	3802	CG1	ILE	498	84.077	-1.006	3.830	1.00	53.85
ATOM	3803	CD1	ILE	498	83.411	0.254	3.271	1.00	55.62
ATOM	3804	C	ILE	498	84.702	-0.802	7.654	1.00	52.74
ATOM	3805	O	ILE	498	85.133	0.293	8.026	1.00	52.14
ATOM	3806	N	GLY	499	84.835	-1.926	8.354	1.00	52.58
ATOM	3808	CA	GLY	499	85.600	-1.974	9.592	1.00	53.03
ATOM	3809	C	GLY	499	85.165	-1.113	10.771	1.00	53.67
ATOM	3810	O	GLY	499	86.012	-0.544	11.463	1.00	53.99
ATOM	3811	N	LEU	500	83.862	-1.045	11.034	1.00	53.60
ATOM	3813	CA	LEU	500	83.337	-0.245	12.141	1.00	51.00
ATOM	3814	CB	LEU	500	81.841	-0.499	12.317	1.00	49.38
ATOM	3815	CG	LEU	500	80.901	-0.024	11.212	1.00	47.62
ATOM	3816	CD1	LEU	500	79.483	-0.454	11.543	1.00	47.25
ATOM	3817	CD2	LEU	500	80.992	1.486	11.081	1.00	47.38
ATOM	3818	C	LEU	500	84.060	-0.573	13.433	1.00	51.05
ATOM	3819	O	LEU	500	84.396	-1.734	13.670	1.00	53.76
ATOM	3820	N	PRO	505	87.588	-5.968	10.545	1.00	81.81
ATOM	3821	CD	PRO	505	88.588	-6.677	11.357	1.00	81.96
ATOM	3822	CA	PRO	505	88.105	-4.664	10.109	1.00	80.56
ATOM	3823	CB	PRO	505	89.501	-4.622	10.735	1.00	80.75
ATOM	3824	CG	PRO	505	89.868	-6.070	10.860	1.00	82.32
ATOM	3825	C	PRO	505	88.139	-4.477	8.588	1.00	78.53
ATOM	3826	O	PRO	505	88.462	-3.400	8.085	1.00	77.85
ATOM	3827	N	ASN	506	87.792	-5.532	7.865	1.00	77.09
ATOM	3829	CA	ASN	506	87.747	-5.484	6.411	1.00	75.57
ATOM	3830	CB	ASN	506	88.799	-6.415	5.806	1.00	75.80
ATOM	3831	C	ASN	506	86.347	-5.929	6.008	1.00	74.33
ATOM	3832	O	ASN	506	86.044	-6.117	4.826	1.00	73.76
ATOM	3833	N	ARG	507	85.496	-6.092	7.018	1.00	71.72
ATOM	3835	CA	ARG	507	84.120	-6.509	6.820	1.00	69.28
ATOM	3836	CB	ARG	507	83.619	-7.257	8.054	1.00	70.64
ATOM	3837	C	ARG	507	83.258	-5.284	6.605	1.00	65.87
ATOM	3838	O	ARG	507	83.445	-4.262	7.274	1.00	65.40
ATOM	3839	N	VAL	508	82.363	-5.358	5.628	1.00	62.01
ATOM	3841	CA	VAL	508	81.464	-4.248	5.381	1.00	58.41
ATOM	3842	CB	VAL	508	81.043	-4.136	3.915	1.00	57.18
ATOM	3843	CG1	VAL	508	82.251	-3.893	3.046	1.00	61.04

ATOM	3844	CG2	VAL	508	80.310	-5.383	3.466	1.00	60.74
ATOM	3845	C	VAL	508	80.257	-4.552	6.246	1.00	56.61
ATOM	3846	O	VAL	508	79.964	-5.716	6.529	1.00	55.82
ATOM	3847	N	THR	509	79.572	-3.501	6.665	1.00	54.85
ATOM	3849	CA	THR	509	78.396	-3.610	7.501	1.00	49.28
ATOM	3850	CB	THR	509	78.705	-3.144	8.934	1.00	47.98
ATOM	3851	OG1	THR	509	79.938	-3.727	9.356	1.00	43.39
ATOM	3853	CG2	THR	509	77.606	-3.565	9.903	1.00	47.57
ATOM	3854	C	THR	509	77.381	-2.674	6.865	1.00	46.71
ATOM	3855	O	THR	509	77.675	-1.507	6.625	1.00	48.59
ATOM	3856	N	LYS	510	76.238	-3.208	6.470	1.00	44.75
ATOM	3858	CA	LYS	510	75.202	-2.372	5.889	1.00	44.42
ATOM	3859	CB	LYS	510	74.069	-3.259	5.365	1.00	46.34
ATOM	3860	CG	LYS	510	73.226	-2.622	4.284	1.00	54.93
ATOM	3861	CD	LYS	510	73.825	-2.807	2.899	1.00	58.33
ATOM	3862	CE	LYS	510	73.118	-3.931	2.152	1.00	59.17
ATOM	3863	NZ	LYS	510	73.317	-5.251	2.813	1.00	56.09
ATOM	3867	C	LYS	510	74.734	-1.499	7.075	1.00	40.83
ATOM	3868	O	LYS	510	74.480	-2.020	8.162	1.00	38.59
ATOM	3869	N	VAL	511	74.679	-0.183	6.891	1.00	36.28
ATOM	3871	CA	VAL	511	74.265	0.720	7.957	1.00	31.41
ATOM	3872	CB	VAL	511	75.480	1.389	8.690	1.00	32.80
ATOM	3873	CG1	VAL	511	76.315	0.346	9.420	1.00	29.97
ATOM	3874	CG2	VAL	511	76.353	2.175	7.706	1.00	30.20
ATOM	3875	C	VAL	511	73.408	1.812	7.360	1.00	28.40
ATOM	3876	O	VAL	511	73.305	1.914	6.147	1.00	27.45
ATOM	3877	N	ALA	512	72.756	2.598	8.207	1.00	27.30
ATOM	3879	CA	ALA	512	71.953	3.701	7.715	1.00	26.66
ATOM	3880	CB	ALA	512	70.557	3.640	8.278	1.00	24.24
ATOM	3881	C	ALA	512	72.670	4.965	8.173	1.00	28.52
ATOM	3882	O	ALA	512	73.140	5.036	9.319	1.00	26.66
ATOM	3883	N	VAL	513	72.768	5.949	7.275	1.00	29.18
ATOM	3885	CA	VAL	513	73.442	7.217	7.569	1.00	29.65
ATOM	3886	CB	VAL	513	74.631	7.482	6.601	1.00	28.93
ATOM	3887	CG1	VAL	513	75.384	8.722	7.015	1.00	25.51
ATOM	3888	CG2	VAL	513	75.570	6.292	6.550	1.00	29.45
ATOM	3889	C	VAL	513	72.509	8.407	7.476	1.00	30.45
ATOM	3890	O	VAL	513	71.900	8.646	6.431	1.00	30.15
ATOM	3891	N	LYS	514	72.402	9.143	8.578	1.00	33.29
ATOM	3893	CA	LYS	514	71.575	10.357	8.654	1.00	33.28
ATOM	3894	CB	LYS	514	71.017	10.537	10.068	1.00	38.67
ATOM	3895	CG	LYS	514	70.074	9.456	10.531	1.00	45.73
ATOM	3896	CD	LYS	514	69.462	9.860	11.855	1.00	53.93
ATOM	3897	CE	LYS	514	68.450	8.840	12.337	1.00	63.59
ATOM	3898	NZ	LYS	514	67.206	8.823	11.517	1.00	71.90
ATOM	3902	C	LYS	514	72.451	11.568	8.312	1.00	29.45
ATOM	3903	O	LYS	514	73.584	11.673	8.794	1.00	25.64
ATOM	3904	N	MET	515	71.918	12.495	7.522	1.00	29.42
ATOM	3906	CA	MET	515	72.668	13.690	7.119	1.00	30.46
ATOM	3907	CB	MET	515	73.464	13.391	5.846	1.00	29.63
ATOM	3908	CG	MET	515	72.557	13.070	4.665	1.00	32.48
ATOM	3909	SD	MET	515	73.391	12.475	3.218	1.00	33.06

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ATOM	3910	CE	MET	515	73.734	10.809	3.715	1.00	30.26
ATOM	3911	C	MET	515	71.700	14.839	6.848	1.00	30.75
ATOM	3912	O	MET	515	70.478	14.654	6.867	1.00	33.07
ATOM	3913	N	LEU	516	72.238	16.027	6.608	1.00	30.32
ATOM	3915	CA	LEU	516	71.414	17.194	6.304	1.00	30.21
ATOM	3916	CB	LEU	516	72.112	18.487	6.748	1.00	26.54
ATOM	3917	CG	LEU	516	72.452	18.668	8.227	1.00	23.97
ATOM	3918	CD1	LEU	516	73.345	19.858	8.412	1.00	24.27
ATOM	3919	CD2	LEU	516	71.198	18.850	9.023	1.00	21.46
ATOM	3920	C	LEU	516	71.197	17.265	4.800	1.00	33.44
ATOM	3921	O	LEU	516	72.016	16.784	4.015	1.00	34.50
ATOM	3922	N	LYS	517	70.082	17.863	4.400	1.00	36.36
ATOM	3924	CA	LYS	517	69.783	18.048	2.993	1.00	34.58
ATOM	3925	CB	LYS	517	68.281	18.255	2.784	1.00	38.96
ATOM	3926	CG	LYS	517	67.409	17.155	3.380	1.00	44.34
ATOM	3927	CD	LYS	517	66.128	16.920	2.572	1.00	52.11
ATOM	3928	CE	LYS	517	65.138	18.083	2.637	1.00	58.29
ATOM	3929	NZ	LYS	517	63.915	17.833	1.786	1.00	60.90
ATOM	3933	C	LYS	517	70.567	19.304	2.597	1.00	33.51
ATOM	3934	O	LYS	517	71.024	20.064	3.460	1.00	30.34
ATOM	3935	N	SER	518	70.701	19.539	1.296	1.00	34.39
ATOM	3937	CA	SER	518	71.444	20.693	0.788	1.00	35.84
ATOM	3938	CB	SER	518	71.537	20.618	-0.731	1.00	33.66
ATOM	3939	OG	SER	518	70.282	20.258	-1.266	1.00	38.73
ATOM	3941	C	SER	518	70.879	22.045	1.198	1.00	36.91
ATOM	3942	O	SER	518	71.591	23.050	1.205	1.00	37.32
ATOM	3943	N	ASP	519	69.598	22.069	1.538	1.00	37.88
ATOM	3945	CA	ASP	519	68.945	23.313	1.936	1.00	38.63
ATOM	3946	CB	ASP	519	67.517	23.364	1.375	1.00	42.23
ATOM	3947	CG	ASP	519	66.669	22.151	1.775	1.00	48.87
ATOM	3948	OD1	ASP	519	67.070	21.380	2.681	1.00	49.21
ATOM	3949	OD2	ASP	519	65.582	21.972	1.181	1.00	54.93
ATOM	3950	C	ASP	519	68.916	23.537	3.443	1.00	38.06
ATOM	3951	O	ASP	519	68.246	24.451	3.916	1.00	39.38
ATOM	3952	N	ALA	520	69.622	22.692	4.191	1.00	36.24
ATOM	3954	CA	ALA	520	69.631	22.795	5.648	1.00	34.69
ATOM	3955	CB	ALA	520	70.359	21.613	6.259	1.00	35.68
ATOM	3956	C	ALA	520	70.213	24.087	6.173	1.00	33.54
ATOM	3957	O	ALA	520	71.039	24.718	5.522	1.00	34.83
ATOM	3958	N	THR	521	69.815	24.452	7.384	1.00	34.45
ATOM	3960	CA	THR	521	70.315	25.668	8.001	1.00	36.51
ATOM	3961	CB	THR	521	69.148	26.592	8.493	1.00	39.14
ATOM	3962	OG1	THR	521	68.529	26.031	9.659	1.00	41.61
ATOM	3964	CG2	THR	521	68.081	26.750	7.409	1.00	40.14
ATOM	3965	C	THR	521	71.228	25.303	9.170	1.00	36.35
ATOM	3966	O	THR	521	71.376	24.125	9.510	1.00	32.23
ATOM	3967	N	GLU	522	71.868	26.310	9.756	1.00	39.33
ATOM	3969	CA	GLU	522	72.747	26.092	10.890	1.00	44.59
ATOM	3970	CB	GLU	522	73.364	27.424	11.335	1.00	51.80
ATOM	3971	CG	GLU	522	74.463	27.311	12.418	1.00	64.10
ATOM	3972	CD	GLU	522	75.811	26.815	11.886	1.00	69.12
ATOM	3973	OE1	GLU	522	76.784	27.605	11.869	1.00	69.26

ATOM	3974	OE2	GLU	522	75.900	25.629	11.502	1.00	73.62
ATOM	3975	C	GLU	522	71.953	25.447	12.042	1.00	44.53
ATOM	3976	O	GLU	522	72.482	24.617	12.786	1.00	44.95
ATOM	3977	N	LYS	523	70.679	25.814	12.167	1.00	42.99
ATOM	3979	CA	LYS	523	69.826	25.264	13.216	1.00	42.17
ATOM	3980	CB	LYS	523	68.519	26.053	13.329	1.00	45.99
ATOM	3981	CG	LYS	523	67.583	25.582	14.433	1.00	48.74
ATOM	3982	CD	LYS	523	66.296	25.027	13.832	1.00	57.24
ATOM	3983	CE	LYS	523	65.405	24.383	14.884	1.00	60.31
ATOM	3984	NZ	LYS	523	64.309	23.586	14.247	1.00	65.17
ATOM	3988	C	LYS	523	69.563	23.793	12.935	1.00	39.03
ATOM	3989	O	LYS	523	69.581	22.973	13.850	1.00	40.65
ATOM	3990	N	ASP	524	69.331	23.457	11.672	1.00	34.91
ATOM	3992	CA	ASP	524	69.122	22.068	11.294	1.00	33.12
ATOM	3993	CB	ASP	524	68.876	21.942	9.790	1.00	34.84
ATOM	3994	CG	ASP	524	67.482	22.352	9.389	1.00	36.47
ATOM	3995	OD1	ASP	524	66.552	22.193	10.204	1.00	41.59
ATOM	3996	OD2	ASP	524	67.307	22.815	8.248	1.00	38.19
ATOM	3997	C	ASP	524	70.383	21.284	11.653	1.00	33.94
ATOM	3998	O	ASP	524	70.301	20.154	12.139	1.00	37.40
ATOM	3999	N	LEU	525	71.554	21.869	11.404	1.00	32.39
ATOM	4001	CA	LEU	525	72.799	21.186	11.729	1.00	31.50
ATOM	4002	CB	LEU	525	74.018	21.998	11.278	1.00	29.05
ATOM	4003	CG	LEU	525	75.363	21.375	11.680	1.00	28.38
ATOM	4004	CD1	LEU	525	75.521	19.990	11.065	1.00	27.27
ATOM	4005	CD2	LEU	525	76.519	22.283	11.295	1.00	26.26
ATOM	4006	C	LEU	525	72.848	20.941	13.231	1.00	30.27
ATOM	4007	O	LEU	525	73.104	19.828	13.675	1.00	33.58
ATOM	4008	N	SER	526	72.563	21.982	14.000	1.00	29.63
ATOM	4010	CA	SER	526	72.544	21.914	15.459	1.00	30.26
ATOM	4011	CB	SER	526	72.046	23.251	16.013	1.00	32.03
ATOM	4012	OG	SER	526	71.923	23.199	17.417	1.00	37.02
ATOM	4014	C	SER	526	71.640	20.796	15.980	1.00	29.72
ATOM	4015	O	SER	526	71.924	20.162	16.998	1.00	27.54
ATOM	4016	N	ASP	527	70.525	20.588	15.291	1.00	28.97
ATOM	4018	CA	ASP	527	69.581	19.556	15.664	1.00	29.28
ATOM	4019	CB	ASP	527	68.289	19.710	14.855	1.00	29.08
ATOM	4020	CG	ASP	527	67.497	20.977	15.225	1.00	30.05
ATOM	4021	OD1	ASP	527	67.750	21.597	16.292	1.00	24.32
ATOM	4022	OD2	ASP	527	66.591	21.335	14.436	1.00	34.69
ATOM	4023	C	ASP	527	70.175	18.164	15.436	1.00	30.65
ATOM	4024	O	ASP	527	70.115	17.297	16.312	1.00	30.12
ATOM	4025	N	LEU	528	70.769	17.958	14.265	1.00	30.50
ATOM	4027	CA	LEU	528	71.358	16.669	13.946	1.00	29.54
ATOM	4028	CB	LEU	528	71.850	16.647	12.487	1.00	26.03
ATOM	4029	CG	LEU	528	72.409	15.320	11.942	1.00	24.26
ATOM	4030	CD1	LEU	528	71.466	14.142	12.259	1.00	21.51
ATOM	4031	CD2	LEU	528	72.644	15.437	10.450	1.00	15.05
ATOM	4032	C	LEU	528	72.494	16.342	14.933	1.00	30.51
ATOM	4033	O	LEU	528	72.641	15.192	15.354	1.00	29.79
ATOM	4034	N	ILE	529	73.281	17.351	15.305	1.00	30.86
ATOM	4036	CA	ILE	529	74.367	17.138	16.253	1.00	28.41

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ATOM	4037	CB	ILE	529	75.266	18.349	16.406	1.00	24.75	
ATOM	4038	CG2	ILE	529	76.355	18.064	17.432	1.00	25.51	
ATOM	4039	CG1	ILE	529	75.901	18.710	15.084	1.00	17.82	
ATOM	4040	CD1	ILE	529	76.912	19.806	15.251	1.00	18.14	
ATOM	4041	C	ILE	529	73.821	16.813	17.641	1.00	30.17	
ATOM	4042	O	ILE	529	74.286	15.873	18.285	1.00	30.11	
ATOM	4043	N	SER	530	72.836	17.574	18.101	1.00	30.29	
ATOM	4045	CA	SER	530	72.271	17.310	19.418	1.00	33.14	
ATOM	4046	CB	SER	530	71.158	18.293	19.735	1.00	36.09	
ATOM	4047	OG	SER	530	70.224	18.323	18.670	1.00	49.01	
ATOM	4049	C	SER	530	71.740	15.881	19.479	1.00	33.80	
ATOM	4050	O	SER	530	71.896	15.190	20.492	1.00	37.06	
ATOM	4051	N	GLU	531	71.156	15.413	18.378	1.00	30.13	
ATOM	4053	CA	GLU	531	70.629	14.065	18.351	1.00	29.18	
ATOM	4054	CB	GLU	531	69.822	13.801	17.087	1.00	32.42	
ATOM	4055	CG	GLU	531	69.253	12.394	17.058	1.00	33.35	
ATOM	4056	CD	GLU	531	68.354	12.131	15.883	1.00	34.76	
ATOM	4057	OE1	GLU	531	67.481	11.249	16.002	1.00	40.42	
ATOM	4058	OE2	GLU	531	68.516	12.793	14.847	1.00	35.88	
ATOM	4059	C	GLU	531	71.734	13.025	18.488	1.00	28.27	
ATOM	4060	O	GLU	531	71.569	12.032	19.192	1.00	26.75	
ATOM	4061	N	MET	532	72.842	13.235	17.786	1.00	27.80	
ATOM	4063	CA	MET	532	73.976	12.320	17.835	1.00	27.82	
ATOM	4064	CB	MET	532	75.080	12.813	16.890	1.00	29.43	
ATOM	4065	CG	MET	532	76.461	12.225	17.138	1.00	24.34	
ATOM	4066	SD	MET	532	77.641	12.702	15.840	1.00	27.83	
ATOM	4067	CE	MET	532	77.791	14.462	16.193	1.00	21.90	
ATOM	4068	C	MET	532	74.499	12.272	19.260	1.00	29.53	
ATOM	4069	O	MET	532	74.742	11.197	19.809	1.00	30.14	
ATOM	4070	N	GLU	533	74.610	13.445	19.871	1.00	30.25	
ATOM	4072	CA	GLU	533	75.109	13.570	21.233	1.00	31.95	
ATOM	4073	CB	GLU	533	75.300	15.039	21.594	1.00	32.55	
ATOM	4074	CG	GLU	533	76.391	15.724	20.765	1.00	35.71	
ATOM	4075	CD	GLU	533	77.766	15.087	20.951	1.00	36.71	
ATOM	4076	OE1	GLU	533	78.297	15.136	22.084	1.00	40.19	
ATOM	4077	OE2	GLU	533	78.322	14.555	19.969	1.00	33.99	
ATOM	4078	C	GLU	533	74.185	12.886	22.225	1.00	33.06	
ATOM	4079	O	GLU	533	74.642	12.197	23.147	1.00	33.49	
ATOM	4080	N	MET	534	72.883	13.052	22.025	1.00	33.12	
ATOM	4082	CA	MET	534	71.913	12.432	22.900	1.00	32.48	
ATOM	4083	CB	MET	534	70.484	12.859	22.533	1.00	30.60	
ATOM	4084	CG	MET	534	69.591	12.915	23.791	0.50	28.70	PRT1
ATOM	4085	SD	MET	534	67.787	12.849	23.608	0.50	27.55	PRT1
ATOM	4086	CE	MET	534	67.409	14.560	23.291	0.50	26.84	PRT1
ATOM	4087	C	MET	534	72.102	10.908	22.785	1.00	31.10	
ATOM	4088	O	MET	534	72.258	10.224	23.791	1.00	32.80	
ATOM	4089	N	MET	535	72.194	10.394	21.563	1.00	30.50	
ATOM	4091	CA	MET	535	72.399	8.961	21.368	1.00	29.25	
ATOM	4092	CB	MET	535	72.577	8.623	19.884	1.00	28.10	
ATOM	4093	CG	MET	535	71.337	8.876	19.042	1.00	27.48	
ATOM	4094	SD	MET	535	71.377	7.980	17.502	1.00	26.94	
ATOM	4095	CE	MET	535	71.346	9.275	16.310	1.00	33.72	

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ATOM	4096	C	MET	535	73.621	8.514	22.155	1.00	29.29
ATOM	4097	O	MET	535	73.640	7.412	22.710	1.00	29.06
ATOM	4098	N	LYS	536	74.644	9.367	22.185	1.00	31.75
ATOM	4100	CA	LYS	536	75.869	9.073	22.930	1.00	33.24
ATOM	4101	CB	LYS	536	76.950	10.108	22.628	1.00	31.29
ATOM	4102	CG	LYS	536	77.602	10.007	21.258	1.00	31.09
ATOM	4103	CD	LYS	536	78.570	11.154	21.103	1.00	28.76
ATOM	4104	CE	LYS	536	79.219	11.220	19.755	1.00	26.70
ATOM	4105	NZ	LYS	536	80.059	12.461	19.742	1.00	27.38
ATOM	4109	C	LYS	536	75.630	9.014	24.451	1.00	35.30
ATOM	4110	O	LYS	536	76.201	8.172	25.137	1.00	35.61
ATOM	4111	N	MET	537	74.788	9.902	24.972	1.00	35.67
ATOM	4113	CA	MET	537	74.517	9.908	26.408	1.00	38.27
ATOM	4114	CB	MET	537	73.858	11.221	26.844	1.00	43.86
ATOM	4115	CG	MET	537	74.801	12.420	26.884	1.00	55.46
ATOM	4116	SD	MET	537	76.189	12.272	28.062	1.00	63.44
ATOM	4117	CE	MET	537	75.383	12.822	29.591	1.00	62.14
ATOM	4118	C	MET	537	73.657	8.734	26.845	1.00	37.10
ATOM	4119	O	MET	537	73.855	8.188	27.920	1.00	39.26
ATOM	4120	N	ILE	538	72.723	8.320	26.003	1.00	34.96
ATOM	4122	CA	ILE	538	71.819	7.219	26.320	1.00	32.78
ATOM	4123	CB	ILE	538	70.618	7.202	25.342	1.00	32.48
ATOM	4124	CG2	ILE	538	69.782	5.943	25.537	1.00	32.27
ATOM	4125	CG1	ILE	538	69.756	8.449	25.538	1.00	31.77
ATOM	4126	CD1	ILE	538	68.746	8.651	24.409	1.00	34.25
ATOM	4127	C	ILE	538	72.456	5.823	26.365	1.00	30.54
ATOM	4128	O	ILE	538	72.146	5.039	27.250	1.00	33.37
ATOM	4129	N	GLY	539	73.293	5.481	25.399	1.00	27.09
ATOM	4131	CA	GLY	539	73.892	4.162	25.419	1.00	28.72
ATOM	4132	C	GLY	539	73.173	3.135	24.552	1.00	31.16
ATOM	4133	O	GLY	539	72.069	3.379	24.060	1.00	32.94
ATOM	4134	N	LYS	540	73.808	1.981	24.370	1.00	31.68
ATOM	4136	CA	LYS	540	73.264	0.912	23.537	1.00	34.64
ATOM	4137	CB	LYS	540	74.399	0.032	23.029	1.00	33.47
ATOM	4138	CG	LYS	540	75.331	0.730	22.095	1.00	39.67
ATOM	4139	CD	LYS	540	76.396	-0.209	21.573	1.00	41.48
ATOM	4140	CE	LYS	540	77.228	0.475	20.501	1.00	48.72
ATOM	4141	NZ	LYS	540	76.442	0.800	19.254	1.00	54.86
ATOM	4145	C	LYS	540	72.206	-0.010	24.143	1.00	36.68
ATOM	4146	O	LYS	540	72.276	-0.370	25.324	1.00	41.03
ATOM	4147	N	HIS	541	71.233	-0.396	23.319	1.00	35.61
ATOM	4149	CA	HIS	541	70.190	-1.335	23.711	1.00	34.24
ATOM	4150	CB	HIS	541	69.074	-0.702	24.526	1.00	33.44
ATOM	4151	CG	HIS	541	68.118	-1.711	25.083	1.00	34.60
ATOM	4152	CD2	HIS	541	68.059	-2.310	26.292	1.00	33.77
ATOM	4153	ND1	HIS	541	67.143	-2.316	24.309	1.00	34.19
ATOM	4155	CE1	HIS	541	66.539	-3.248	25.020	1.00	36.87
ATOM	4156	NE2	HIS	541	67.074	-3.272	26.228	1.00	34.05
ATOM	4158	C	HIS	541	69.624	-2.023	22.474	1.00	36.31
ATOM	4159	O	HIS	541	69.342	-1.378	21.457	1.00	38.40
ATOM	4160	N	LYS	542	69.407	-3.331	22.586	1.00	36.42
ATOM	4162	CA	LYS	542	68.923	-4.155	21.469	1.00	35.10



ATOM	4163	CB	LYS	542	68.680	-5.602	21.915	1.00	34.24
ATOM	4164	C	LYS	542	67.674	-3.646	20.802	1.00	32.40
ATOM	4165	O	LYS	542	67.507	-3.822	19.612	1.00	32.37
ATOM	4166	N	ASN	543	66.785	-3.046	21.580	1.00	32.12
ATOM	4168	CA	ASN	543	65.541	-2.561	21.015	1.00	33.01
ATOM	4169	CB	ASN	543	64.361	-3.081	21.842	1.00	34.26
ATOM	4170	CG	ASN	543	64.365	-4.597	21.979	1.00	32.20
ATOM	4171	OD1	ASN	543	64.633	-5.128	23.050	1.00	32.23
ATOM	4172	ND2	ASN	543	64.077	-5.292	20.904	1.00	30.50
ATOM	4175	C	ASN	543	65.424	-1.050	20.719	1.00	32.21
ATOM	4176	O	ASN	543	64.326	-0.481	20.765	1.00	31.13
ATOM	4177	N	ILE	544	66.556	-0.419	20.397	1.00	30.52
ATOM	4179	CA	ILE	544	66.611	1.002	20.028	1.00	29.01
ATOM	4180	CB	ILE	544	67.040	1.962	21.208	1.00	25.83
ATOM	4181	CG2	ILE	544	66.244	1.682	22.467	1.00	24.46
ATOM	4182	CG1	ILE	544	68.532	1.848	21.522	1.00	27.54
ATOM	4183	CD1	ILE	544	69.008	2.839	22.581	1.00	22.70
ATOM	4184	C	ILE	544	67.617	1.118	18.870	1.00	29.49
ATOM	4185	O	ILE	544	68.410	0.194	18.633	1.00	27.26
ATOM	4186	N	ILE	545	67.504	2.184	18.078	1.00	28.74
ATOM	4188	CA	ILE	545	68.453	2.396	16.992	1.00	27.06
ATOM	4189	CB	ILE	545	67.913	3.350	15.921	1.00	23.64
ATOM	4190	CG2	ILE	545	69.027	3.727	14.955	1.00	23.96
ATOM	4191	CG1	ILE	545	66.754	2.692	15.167	1.00	23.13
ATOM	4192	CD1	ILE	545	67.152	1.481	14.339	1.00	20.61
ATOM	4193	C	ILE	545	69.720	2.968	17.633	1.00	26.93
ATOM	4194	O	ILE	545	69.719	4.075	18.160	1.00	28.63
ATOM	4195	N	ASN	546	70.800	2.200	17.560	1.00	28.53
ATOM	4197	CA	ASN	546	72.075	2.567	18.161	1.00	29.39
ATOM	4198	CB	ASN	546	72.752	1.308	18.718	1.00	29.14
ATOM	4199	CG	ASN	546	71.908	0.613	19.772	1.00	30.21
ATOM	4200	OD1	ASN	546	71.804	1.088	20.899	1.00	30.74
ATOM	4201	ND2	ASN	546	71.290	-0.505	19.406	1.00	30.79
ATOM	4204	C	ASN	546	73.034	3.303	17.238	1.00	30.78
ATOM	4205	O	ASN	546	73.011	3.126	16.015	1.00	33.04
ATOM	4206	N	LEU	547	73.866	4.151	17.837	1.00	31.07
ATOM	4208	CA	LEU	547	74.880	4.904	17.101	1.00	31.37
ATOM	4209	CB	LEU	547	75.284	6.165	17.875	1.00	27.32
ATOM	4210	CG	LEU	547	76.413	7.032	17.297	1.00	24.17
ATOM	4211	CD1	LEU	547	75.953	7.768	16.069	1.00	18.06
ATOM	4212	CD2	LEU	547	76.864	8.014	18.348	1.00	22.50
ATOM	4213	C	LEU	547	76.107	3.999	16.861	1.00	33.38
ATOM	4214	O	LEU	547	76.610	3.343	17.789	1.00	33.58
ATOM	4215	N	LEU	548	76.543	3.919	15.607	1.00	32.72
ATOM	4217	CA	LEU	548	77.694	3.104	15.259	1.00	31.50
ATOM	4218	CB	LEU	548	77.388	2.244	14.029	1.00	26.30
ATOM	4219	CG	LEU	548	76.148	1.341	14.158	1.00	25.93
ATOM	4220	CD1	LEU	548	76.034	0.513	12.906	1.00	28.37
ATOM	4221	CD2	LEU	548	76.196	0.436	15.394	1.00	15.84
ATOM	4222	C	LEU	548	78.941	3.965	15.030	1.00	33.69
ATOM	4223	O	LEU	548	80.063	3.488	15.167	1.00	37.41
ATOM	4224	N	GLY	549	78.746	5.229	14.675	1.00	34.10

ATOM	4226	CA	GLY	549	79.871	6.116	14.454	1.00	31.50
ATOM	4227	C	GLY	549	79.425	7.429	13.839	1.00	31.11
ATOM	4228	O	GLY	549	78.221	7.686	13.700	1.00	30.15
ATOM	4229	N	ALA	550	80.388	8.268	13.474	1.00	31.02
ATOM	4231	CA	ALA	550	80.074	9.540	12.850	1.00	29.00
ATOM	4232	CB	ALA	550	79.537	10.526	13.899	1.00	27.87
ATOM	4233	C	ALA	550	81.257	10.149	12.102	1.00	27.66
ATOM	4234	O	ALA	550	82.422	9.942	12.474	1.00	25.24
ATOM	4235	N	CYS	551	80.944	10.810	10.984	1.00	27.61
ATOM	4237	CA	CYS	551	81.924	11.540	10.170	1.00	25.02
ATOM	4238	CB	CYS	551	81.754	11.237	8.680	1.00	22.41
ATOM	4239	SG	CYS	551	82.155	9.553	8.187	1.00	27.24
ATOM	4240	C	CYS	551	81.583	13.009	10.447	1.00	24.31
ATOM	4241	O	CYS	551	80.569	13.525	9.958	1.00	23.55
ATOM	4242	N	THR	552	82.367	13.657	11.303	1.00	23.22
ATOM	4244	CA	THR	552	82.110	15.046	11.664	1.00	25.73
ATOM	4245	CB	THR	552	82.138	15.215	13.202	1.00	26.50
ATOM	4246	OG1	THR	552	83.479	15.031	13.664	1.00	26.31
ATOM	4248	CG2	THR	552	81.257	14.171	13.886	1.00	26.64
ATOM	4249	C	THR	552	83.134	16.014	11.090	1.00	27.93
ATOM	4250	O	THR	552	82.894	17.216	11.005	1.00	28.35
ATOM	4251	N	GLN	553	84.264	15.473	10.663	1.00	30.26
ATOM	4253	CA	GLN	553	85.355	16.288	10.153	1.00	29.27
ATOM	4254	CB	GLN	553	86.669	15.768	10.763	1.00	29.54
ATOM	4255	CG	GLN	553	86.653	15.655	12.288	1.00	28.00
ATOM	4256	CD	GLN	553	86.534	17.007	12.981	1.00	26.86
ATOM	4257	OE1	GLN	553	87.440	17.821	12.902	1.00	30.85
ATOM	4258	NE2	GLN	553	85.421	17.239	13.676	1.00	23.89
ATOM	4261	C	GLN	553	85.475	16.316	8.634	1.00	28.30
ATOM	4262	O	GLN	553	85.221	15.313	7.967	1.00	31.00
ATOM	4263	N	ASP	554	85.860	17.480	8.119	1.00	26.89
ATOM	4265	CA	ASP	554	86.070	17.725	6.695	1.00	27.85
ATOM	4266	CB	ASP	554	87.370	17.081	6.257	1.00	33.44
ATOM	4267	CG	ASP	554	88.534	17.564	7.060	1.00	37.63
ATOM	4268	OD1	ASP	554	89.038	18.664	6.763	1.00	42.66
ATOM	4269	OD2	ASP	554	88.929	16.843	8.000	1.00	35.80
ATOM	4270	C	ASP	554	84.976	17.341	5.715	1.00	28.04
ATOM	4271	O	ASP	554	85.193	16.518	4.826	1.00	31.06
ATOM	4272	N	GLY	555	83.824	17.981	5.842	1.00	28.26
ATOM	4274	CA	GLY	555	82.720	17.694	4.949	1.00	25.89
ATOM	4275	C	GLY	555	81.438	17.567	5.734	1.00	23.07
ATOM	4276	O	GLY	555	81.423	17.795	6.941	1.00	20.20
ATOM	4277	N	PRO	556	80.338	17.185	5.076	1.00	22.81
ATOM	4278	CD	PRO	556	80.280	16.750	3.679	1.00	22.33
ATOM	4279	CA	PRO	556	79.039	17.032	5.733	1.00	23.99
ATOM	4280	CB	PRO	556	78.154	16.499	4.612	1.00	22.41
ATOM	4281	CG	PRO	556	79.144	15.801	3.698	1.00	24.36
ATOM	4282	C	PRO	556	79.080	16.066	6.911	1.00	26.98
ATOM	4283	O	PRO	556	79.854	15.111	6.934	1.00	28.57
ATOM	4284	N	LEU	557	78.237	16.325	7.896	1.00	29.25
ATOM	4286	CA	LEU	557	78.168	15.471	9.070	1.00	30.83
ATOM	4287	CB	LEU	557	77.550	16.225	10.251	1.00	33.20

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ATOM	4288	CG	LEU	557	77.109	15.416	11.475	1.00	30.01
ATOM	4289	CD1	LEU	557	78.304	14.793	12.174	1.00	29.05
ATOM	4290	CD2	LEU	557	76.365	16.341	12.407	1.00	29.20
ATOM	4291	C	LEU	557	77.324	14.238	8.780	1.00	30.33
ATOM	4292	O	LEU	557	76.175	14.343	8.330	1.00	27.66
ATOM	4293	N	TYR	558	77.913	13.071	9.002	1.00	30.68
ATOM	4295	CA	TYR	558	77.214	11.823	8.812	1.00	29.26
ATOM	4296	CB	TYR	558	77.978	10.933	7.840	1.00	30.99
ATOM	4297	CG	TYR	558	78.066	11.481	6.430	1.00	35.01
ATOM	4298	CD1	TYR	558	79.108	11.109	5.592	1.00	36.17
ATOM	4299	CE1	TYR	558	79.198	11.600	4.296	1.00	41.40
ATOM	4300	CD2	TYR	558	77.109	12.368	5.941	1.00	36.44
ATOM	4301	CE2	TYR	558	77.188	12.871	4.648	1.00	40.96
ATOM	4302	CZ	TYR	558	78.237	12.484	3.825	1.00	43.59
ATOM	4303	OH	TYR	558	78.298	12.965	2.525	1.00	42.91
ATOM	4305	C	TYR	558	77.081	11.125	10.164	1.00	28.18
ATOM	4306	O	TYR	558	78.077	10.855	10.835	1.00	28.06
ATOM	4307	N	VAL	559	75.842	10.879	10.574	1.00	26.72
ATOM	4309	CA	VAL	559	75.548	10.175	11.821	1.00	26.72
ATOM	4310	CB	VAL	559	74.326	10.813	12.552	1.00	28.03
ATOM	4311	CG1	VAL	559	73.915	9.992	13.771	1.00	29.85
ATOM	4312	CG2	VAL	559	74.655	12.236	12.982	1.00	29.37
ATOM	4313	C	VAL	559	75.238	8.723	11.443	1.00	25.58
ATOM	4314	O	VAL	559	74.131	8.402	10.988	1.00	25.73
ATOM	4315	N	ILE	560	76.214	7.851	11.642	1.00	24.35
ATOM	4317	CA	ILE	560	76.061	6.448	11.281	1.00	26.64
ATOM	4318	CB	ILE	560	77.441	5.781	11.002	1.00	26.53
ATOM	4319	CG2	ILE	560	77.252	4.359	10.465	1.00	27.80
ATOM	4320	CG1	ILE	560	78.254	6.620	10.004	1.00	24.69
ATOM	4321	CD1	ILE	560	79.671	6.112	9.763	1.00	17.05
ATOM	4322	C	ILE	560	75.312	5.633	12.339	1.00	27.95
ATOM	4323	O	ILE	560	75.777	5.493	13.479	1.00	25.16
ATOM	4324	N	VAL	561	74.163	5.084	11.951	1.00	27.43
ATOM	4326	CA	VAL	561	73.352	4.265	12.847	1.00	27.69
ATOM	4327	CB	VAL	561	72.048	5.000	13.251	1.00	25.08
ATOM	4328	CG1	VAL	561	72.367	6.302	13.936	1.00	19.97
ATOM	4329	CG2	VAL	561	71.186	5.250	12.033	1.00	25.55
ATOM	4330	C	VAL	561	73.031	2.896	12.202	1.00	30.21
ATOM	4331	O	VAL	561	73.404	2.623	11.045	1.00	32.04
ATOM	4332	N	GLU	562	72.306	2.062	12.944	1.00	28.88
ATOM	4334	CA	GLU	562	71.940	0.714	12.509	1.00	27.69
ATOM	4335	CB	GLU	562	71.448	-0.081	13.712	1.00	26.79
ATOM	4336	CG	GLU	562	72.387	0.001	14.873	1.00	28.13
ATOM	4337	CD	GLU	562	72.012	-0.916	16.003	1.00	31.86
ATOM	4338	OE1	GLU	562	72.772	-1.876	16.255	1.00	33.17
ATOM	4339	OE2	GLU	562	70.974	-0.654	16.639	1.00	35.50
ATOM	4340	C	GLU	562	70.898	0.636	11.405	1.00	27.34
ATOM	4341	O	GLU	562	69.990	1.453	11.358	1.00	29.72
ATOM	4342	N	TYR	563	71.002	-0.392	10.568	1.00	28.07
ATOM	4344	CA	TYR	563	70.080	-0.626	9.455	1.00	32.50
ATOM	4345	CB	TYR	563	70.848	-1.236	8.269	1.00	28.32
ATOM	4346	CG	TYR	563	70.042	-1.427	7.007	1.00	26.56

ATOM	4347	CD1	TYR	563	69.338	-0.378	6.448	1.00	30.49
ATOM	4348	CE1	TYR	563	68.620	-0.536	5.258	1.00	32.83
ATOM	4349	CD2	TYR	563	70.011	-2.652	6.350	1.00	29.07
ATOM	4350	CE2	TYR	563	69.300	-2.821	5.151	1.00	30.70
ATOM	4351	CZ	TYR	563	68.605	-1.755	4.619	1.00	33.54
ATOM	4352	OH	TYR	563	67.876	-1.919	3.460	1.00	40.20
ATOM	4354	C	TYR	563	68.930	-1.564	9.878	1.00	36.30
ATOM	4355	O	TYR	563	69.151	-2.569	10.562	1.00	36.17
ATOM	4356	N	ALA	564	67.711	-1.234	9.454	1.00	39.60
ATOM	4358	CA	ALA	564	66.529	-2.025	9.750	1.00	38.93
ATOM	4359	CB	ALA	564	65.557	-1.207	10.570	1.00	40.23
ATOM	4360	C	ALA	564	65.919	-2.360	8.394	1.00	41.61
ATOM	4361	O	ALA	564	64.958	-1.736	7.977	1.00	45.88
ATOM	4362	N	SER	565	66.455	-3.387	7.745	1.00	41.15
ATOM	4364	CA	SER	565	66.018	-3.806	6.421	1.00	40.40
ATOM	4365	CB	SER	565	66.673	-5.134	6.070	1.00	40.15
ATOM	4366	OG	SER	565	66.646	-6.012	7.175	1.00	33.93
ATOM	4368	C	SER	565	64.530	-3.932	6.164	1.00	40.31
ATOM	4369	O	SER	565	64.097	-3.823	5.025	1.00	45.43
ATOM	4370	N	LYS	566	63.743	-4.183	7.197	1.00	39.63
ATOM	4372	CA	LYS	566	62.312	-4.341	6.992	1.00	38.01
ATOM	4373	CB	LYS	566	61.807	-5.541	7.783	1.00	38.35
ATOM	4374	CG	LYS	566	62.468	-6.828	7.308	1.00	38.21
ATOM	4375	CD	LYS	566	62.161	-8.004	8.208	1.00	38.79
ATOM	4376	CE	LYS	566	62.734	-9.277	7.621	1.00	38.76
ATOM	4377	NZ	LYS	566	62.692	-10.400	8.598	1.00	42.40
ATOM	4381	C	LYS	566	61.488	-3.079	7.249	1.00	37.28
ATOM	4382	O	LYS	566	60.265	-3.132	7.415	1.00	39.48
ATOM	4383	N	GLY	567	62.166	-1.936	7.237	1.00	34.31
ATOM	4385	CA	GLY	567	61.497	-0.666	7.428	1.00	32.82
ATOM	4386	C	GLY	567	60.810	-0.473	8.761	1.00	31.33
ATOM	4387	O	GLY	567	61.251	-1.012	9.778	1.00	29.23
ATOM	4388	N	ASN	568	59.722	0.294	8.754	1.00	29.92
ATOM	4390	CA	ASN	568	58.999	0.569	9.974	1.00	31.05
ATOM	4391	CB	ASN	568	58.414	1.991	9.991	1.00	31.23
ATOM	4392	CG	ASN	568	57.201	2.157	9.087	1.00	34.16
ATOM	4393	OD1	ASN	568	56.095	1.685	9.385	1.00	37.22
ATOM	4394	ND2	ASN	568	57.394	2.877	7.999	1.00	35.13
ATOM	4397	C	ASN	568	57.950	-0.486	10.235	1.00	31.60
ATOM	4398	O	ASN	568	57.535	-1.205	9.324	1.00	31.76
ATOM	4399	N	LEU	569	57.517	-0.548	11.490	1.00	34.63
ATOM	4401	CA	LEU	569	56.540	-1.511	11.979	1.00	35.49
ATOM	4402	CB	LEU	569	56.456	-1.408	13.500	1.00	36.13
ATOM	4403	CG	LEU	569	55.509	-2.363	14.210	1.00	34.78
ATOM	4404	CD1	LEU	569	56.010	-3.804	14.034	1.00	35.01
ATOM	4405	CD2	LEU	569	55.425	-1.971	15.664	1.00	31.13
ATOM	4406	C	LEU	569	55.141	-1.420	11.382	1.00	37.34
ATOM	4407	O	LEU	569	54.518	-2.447	11.141	1.00	41.49
ATOM	4408	N	ARG	570	54.636	-0.213	11.162	1.00	37.19
ATOM	4410	CA	ARG	570	53.299	-0.063	10.591	1.00	39.79
ATOM	4411	CB	ARG	570	52.979	1.403	10.331	1.00	39.48
ATOM	4412	CG	ARG	570	51.558	1.638	9.887	1.00	41.93

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ATOM	4413	CD	ARG	570	51.459	2.966	9.182	1.00	49.89
ATOM	4414	NE	ARG	570	52.329	2.991	8.009	1.00	55.25
ATOM	4416	CZ	ARG	570	53.121	4.008	7.693	1.00	57.90
ATOM	4417	NH1	ARG	570	53.145	5.093	8.455	1.00	56.93
ATOM	4420	NH2	ARG	570	53.921	3.920	6.637	1.00	57.58
ATOM	4423	C	ARG	570	53.219	-0.835	9.278	1.00	39.84
ATOM	4424	O	ARG	570	52.309	-1.644	9.060	1.00	42.48
ATOM	4425	N	GLU	571	54.208	-0.597	8.425	1.00	38.22
ATOM	4427	CA	GLU	571	54.292	-1.251	7.135	1.00	38.84
ATOM	4428	CB	GLU	571	55.284	-0.492	6.266	1.00	40.72
ATOM	4429	CG	GLU	571	54.818	0.941	5.999	1.00	49.17
ATOM	4430	CD	GLU	571	55.845	1.798	5.284	1.00	58.95
ATOM	4431	OE1	GLU	571	57.047	1.434	5.278	1.00	67.07
ATOM	4432	OE2	GLU	571	55.455	2.854	4.736	1.00	61.02
ATOM	4433	C	GLU	571	54.617	-2.744	7.240	1.00	37.79
ATOM	4434	O	GLU	571	54.075	-3.558	6.488	1.00	37.63
ATOM	4435	N	TYR	572	55.462	-3.104	8.204	1.00	36.89
ATOM	4437	CA	TYR	572	55.841	-4.498	8.437	1.00	36.81
ATOM	4438	CB	TYR	572	56.822	-4.584	9.612	1.00	33.24
ATOM	4439	CG	TYR	572	57.191	-5.987	10.080	1.00	33.42
ATOM	4440	CD1	TYR	572	58.209	-6.714	9.450	1.00	31.93
ATOM	4441	CE1	TYR	572	58.623	-7.960	9.936	1.00	30.14
ATOM	4442	CD2	TYR	572	56.586	-6.552	11.208	1.00	34.42
ATOM	4443	CE2	TYR	572	56.991	-7.799	11.704	1.00	32.29
ATOM	4444	CZ	TYR	572	58.012	-8.495	11.065	1.00	32.52
ATOM	4445	OH	TYR	572	58.427	-9.717	11.571	1.00	31.70
ATOM	4447	C	TYR	572	54.588	-5.310	8.754	1.00	37.64
ATOM	4448	O	TYR	572	54.387	-6.410	8.226	1.00	35.70
ATOM	4449	N	LEU	573	53.742	-4.740	9.608	1.00	38.63
ATOM	4451	CA	LEU	573	52.498	-5.376	10.011	1.00	38.21
ATOM	4452	CB	LEU	573	51.802	-4.532	11.067	1.00	35.40
ATOM	4453	CG	LEU	573	52.494	-4.421	12.419	1.00	34.55
ATOM	4454	CD1	LEU	573	51.755	-3.402	13.258	1.00	32.02
ATOM	4455	CD2	LEU	573	52.537	-5.788	13.108	1.00	34.58
ATOM	4456	C	LEU	573	51.570	-5.549	8.818	1.00	38.11
ATOM	4457	O	LEU	573	51.144	-6.656	8.507	1.00	37.68
ATOM	4458	N	GLN	574	51.286	-4.448	8.138	1.00	40.92
ATOM	4460	CA	GLN	574	50.402	-4.476	6.982	1.00	45.16
ATOM	4461	CB	GLN	574	50.213	-3.071	6.447	1.00	44.16
ATOM	4462	CG	GLN	574	49.380	-2.239	7.369	1.00	45.26
ATOM	4463	CD	GLN	574	49.222	-0.849	6.863	1.00	47.09
ATOM	4464	OE1	GLN	574	49.789	-0.483	5.838	1.00	50.83
ATOM	4465	NE2	GLN	574	48.450	-0.051	7.573	1.00	48.95
ATOM	4468	C	GLN	574	50.807	-5.419	5.861	1.00	45.21
ATOM	4469	O	GLN	574	49.951	-6.031	5.215	1.00	49.63
ATOM	4470	N	ALA	575	52.105	-5.562	5.646	1.00	43.35
ATOM	4472	CA	ALA	575	52.579	-6.446	4.604	1.00	42.62
ATOM	4473	CB	ALA	575	54.023	-6.130	4.284	1.00	43.49
ATOM	4474	C	ALA	575	52.439	-7.906	5.022	1.00	42.85
ATOM	4475	O	ALA	575	52.771	-8.804	4.254	1.00	44.43
ATOM	4476	N	ARG	576	51.937	-8.142	6.229	1.00	42.24
ATOM	4478	CA	ARG	576	51.787	-9.494	6.747	1.00	41.58

ATOM	4479	CB	ARG	576	52.813	-9.725	7.849	1.00	40.10
ATOM	4480	CG	ARG	576	54.225	-9.694	7.314	1.00	40.58
ATOM	4481	CD	ARG	576	55.280	-9.604	8.392	1.00	42.40
ATOM	4482	NE	ARG	576	56.632	-9.607	7.826	1.00	41.95
ATOM	4484	CZ	ARG	576	57.110	-8.684	6.992	1.00	38.22
ATOM	4485	NH1	ARG	576	56.359	-7.658	6.612	1.00	38.61
ATOM	4488	NH2	ARG	576	58.347	-8.787	6.541	1.00	34.50
ATOM	4491	C	ARG	576	50.389	-9.762	7.255	1.00	43.28
ATOM	4492	O	ARG	576	50.187	-10.607	8.137	1.00	43.76
ATOM	4493	N	ARG	577	49.418	-9.057	6.684	1.00	44.65
ATOM	4495	CA	ARG	577	48.023	-9.222	7.077	1.00	46.69
ATOM	4496	CB	ARG	577	47.197	-8.032	6.587	1.00	45.24
ATOM	4497	CG	ARG	577	47.372	-6.793	7.440	1.00	42.93
ATOM	4498	CD	ARG	577	46.572	-5.635	6.898	1.00	44.63
ATOM	4499	NE	ARG	577	46.428	-4.577	7.895	1.00	47.76
ATOM	4501	CZ	ARG	577	45.750	-3.450	7.704	1.00	48.55
ATOM	4502	NH1	ARG	577	45.149	-3.225	6.548	1.00	50.64
ATOM	4505	NH2	ARG	577	45.643	-2.560	8.684	1.00	50.77
ATOM	4508	C	ARG	577	47.408	-10.540	6.603	1.00	47.12
ATOM	4509	O	ARG	577	47.396	-10.840	5.406	1.00	48.37
ATOM	4510	N	GLN	594	53.246	-13.695	7.891	1.00	64.66
ATOM	4512	CA	GLN	594	52.054	-13.835	8.728	1.00	65.10
ATOM	4513	CB	GLN	594	51.130	-14.931	8.184	1.00	65.77
ATOM	4514	C	GLN	594	52.447	-14.127	10.174	1.00	64.01
ATOM	4515	O	GLN	594	52.962	-15.201	10.507	1.00	64.42
ATOM	4516	N	LEU	595	52.189	-13.154	11.031	1.00	61.45
ATOM	4518	CA	LEU	595	52.524	-13.245	12.437	1.00	59.21
ATOM	4519	CB	LEU	595	52.669	-11.826	12.979	1.00	57.54
ATOM	4520	CG	LEU	595	53.648	-11.043	12.099	1.00	56.37
ATOM	4521	CD1	LEU	595	53.442	-9.551	12.202	1.00	57.06
ATOM	4522	CD2	LEU	595	55.064	-11.430	12.465	1.00	55.57
ATOM	4523	C	LEU	595	51.509	-14.046	13.257	1.00	58.34
ATOM	4524	O	LEU	595	50.316	-14.039	12.953	1.00	58.21
ATOM	4525	N	SER	596	52.007	-14.740	14.280	1.00	58.00
ATOM	4527	CA	SER	596	51.182	-15.543	15.180	1.00	56.04
ATOM	4528	CB	SER	596	51.960	-16.770	15.667	1.00	57.98
ATOM	4529	OG	SER	596	52.987	-16.403	16.580	1.00	58.94
ATOM	4531	C	SER	596	50.854	-14.681	16.383	1.00	54.65
ATOM	4532	O	SER	596	51.479	-13.645	16.584	1.00	52.05
ATOM	4533	N	SER	597	49.914	-15.133	17.208	1.00	56.10
ATOM	4535	CA	SER	597	49.525	-14.389	18.398	1.00	57.51
ATOM	4536	CB	SER	597	48.530	-15.196	19.236	1.00	58.60
ATOM	4537	OG	SER	597	47.620	-15.914	18.421	1.00	61.95
ATOM	4539	C	SER	597	50.778	-14.094	19.220	1.00	57.75
ATOM	4540	O	SER	597	50.934	-12.998	19.755	1.00	57.86
ATOM	4541	N	LYS	598	51.692	-15.062	19.271	1.00	57.88
ATOM	4543	CA	LYS	598	52.930	-14.905	20.026	1.00	57.51
ATOM	4544	CB	LYS	598	53.690	-16.231	20.124	1.00	57.72
ATOM	4545	CG	LYS	598	54.470	-16.395	21.432	1.00	60.14
ATOM	4546	CD	LYS	598	55.227	-17.724	21.479	1.00	62.23
ATOM	4547	CE	LYS	598	55.894	-17.989	22.834	1.00	60.79
ATOM	4548	NZ	LYS	598	54.921	-18.149	23.949	1.00	61.46

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ATOM	4552	C	LYS	598	53.809	-13.829	19.389	1.00	55.94
ATOM	4553	O	LYS	598	54.322	-12.955	20.089	1.00	55.84
ATOM	4554	N	ASP	599	53.935	-13.866	18.061	1.00	53.32
ATOM	4556	CA	ASP	599	54.737	-12.882	17.334	1.00	50.30
ATOM	4557	CB	ASP	599	54.688	-13.119	15.823	1.00	49.72
ATOM	4558	CG	ASP	599	55.426	-14.383	15.394	1.00	53.97
ATOM	4559	OD1	ASP	599	56.176	-14.948	16.214	1.00	58.12
ATOM	4560	OD2	ASP	599	55.261	-14.822	14.233	1.00	55.58
ATOM	4561	C	ASP	599	54.247	-11.474	17.636	1.00	49.53
ATOM	4562	O	ASP	599	55.054	-10.589	17.911	1.00	51.16
ATOM	4563	N	LEU	600	52.930	-11.281	17.634	1.00	47.50
ATOM	4565	CA	LEU	600	52.354	-9.972	17.909	1.00	45.41
ATOM	4566	CB	LEU	600	50.850	-9.948	17.627	1.00	43.77
ATOM	4567	CG	LEU	600	50.429	-10.121	16.169	1.00	41.05
ATOM	4568	CD1	LEU	600	48.941	-9.904	16.048	1.00	41.04
ATOM	4569	CD2	LEU	600	51.160	-9.140	15.294	1.00	39.59
ATOM	4570	C	LEU	600	52.638	-9.485	19.318	1.00	46.77
ATOM	4571	O	LEU	600	52.964	-8.308	19.497	1.00	48.74
ATOM	4572	N	VAL	601	52.524	-10.372	20.314	1.00	47.64
ATOM	4574	CA	VAL	601	52.804	-10.002	21.716	1.00	47.38
ATOM	4575	CB	VAL	601	52.321	-11.070	22.756	1.00	46.58
ATOM	4576	CG1	VAL	601	52.081	-10.403	24.114	1.00	45.07
ATOM	4577	CG2	VAL	601	51.058	-11.759	22.306	1.00	48.86
ATOM	4578	C	VAL	601	54.321	-9.811	21.890	1.00	46.04
ATOM	4579	O	VAL	601	54.793	-8.935	22.622	1.00	46.13
ATOM	4580	N	SER	602	55.090	-10.624	21.183	1.00	44.21
ATOM	4582	CA	SER	602	56.534	-10.546	21.233	1.00	42.78
ATOM	4583	CB	SER	602	57.119	-11.594	20.297	1.00	43.98
ATOM	4584	OG	SER	602	58.523	-11.615	20.355	1.00	51.02
ATOM	4586	C	SER	602	56.954	-9.135	20.813	1.00	41.74
ATOM	4587	O	SER	602	57.709	-8.467	21.524	1.00	44.09
ATOM	4588	N	CYS	603	56.425	-8.667	19.685	1.00	39.57
ATOM	4590	CA	CYS	603	56.699	-7.317	19.177	1.00	36.11
ATOM	4591	CB	CYS	603	55.852	-7.058	17.924	1.00	34.72
ATOM	4592	SG	CYS	603	55.760	-5.364	17.323	0.50	29.10
ATOM	4593	C	CYS	603	56.378	-6.272	20.252	1.00	34.50
ATOM	4594	O	CYS	603	57.174	-5.371	20.506	1.00	33.61
ATOM	4595	N	ALA	604	55.236	-6.429	20.913	1.00	34.64
ATOM	4597	CA	ALA	604	54.811	-5.506	21.964	1.00	37.18
ATOM	4598	CB	ALA	604	53.386	-5.850	22.414	1.00	38.20
ATOM	4599	C	ALA	604	55.786	-5.516	23.160	1.00	38.91
ATOM	4600	O	ALA	604	56.026	-4.481	23.790	1.00	38.29
ATOM	4601	N	TYR	605	56.323	-6.693	23.477	1.00	39.54
ATOM	4603	CA	TYR	605	57.283	-6.854	24.565	1.00	39.29
ATOM	4604	CB	TYR	605	57.573	-8.340	24.791	1.00	40.07
ATOM	4605	CG	TYR	605	58.663	-8.622	25.807	1.00	39.09
ATOM	4606	CD1	TYR	605	58.525	-8.236	27.137	1.00	38.50
ATOM	4607	CE1	TYR	605	59.526	-8.505	28.074	1.00	40.76
ATOM	4608	CD2	TYR	605	59.831	-9.283	25.435	1.00	39.73
ATOM	4609	CE2	TYR	605	60.834	-9.553	26.361	1.00	37.45
ATOM	4610	CZ	TYR	605	60.678	-9.166	27.677	1.00	40.34
ATOM	4611	OH	TYR	605	61.666	-9.466	28.601	1.00	43.16

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ATOM	4613	C	TYR	605	58.582	-6.113	24.224	1.00	39.45
ATOM	4614	O	TYR	605	59.067	-5.291	25.022	1.00	38.75
ATOM	4615	N	GLN	606	59.129	-6.410	23.040	1.00	36.41
ATOM	4617	CA	GLN	606	60.361	-5.787	22.550	1.00	35.20
ATOM	4618	CB	GLN	606	60.695	-6.303	21.150	1.00	34.86
ATOM	4619	CG	GLN	606	61.286	-7.695	21.118	1.00	32.21
ATOM	4620	CD	GLN	606	61.502	-8.205	19.709	1.00	32.63
ATOM	4621	OE1	GLN	606	62.495	-7.888	19.075	1.00	32.16
ATOM	4622	NE2	GLN	606	60.568	-9.004	19.216	1.00	34.62
ATOM	4625	C	GLN	606	60.286	-4.252	22.525	1.00	36.03
ATOM	4626	O	GLN	606	61.209	-3.572	22.989	1.00	38.81
ATOM	4627	N	VAL	607	59.188	-3.716	21.998	1.00	33.45
ATOM	4629	CA	VAL	607	58.979	-2.280	21.923	1.00	29.34
ATOM	4630	CB	VAL	607	57.651	-1.948	21.189	1.00	28.80
ATOM	4631	CG1	VAL	607	57.260	-0.495	21.401	1.00	26.68
ATOM	4632	CG2	VAL	607	57.790	-2.244	19.699	1.00	24.66
ATOM	4633	C	VAL	607	58.965	-1.698	23.339	1.00	31.35
ATOM	4634	O	VAL	607	59.557	-0.643	23.579	1.00	33.86
ATOM	4635	N	ALA	608	58.317	-2.402	24.270	1.00	30.17
ATOM	4637	CA	ALA	608	58.235	-1.971	25.667	1.00	28.98
ATOM	4638	CB	ALA	608	57.255	-2.836	26.440	1.00	28.30
ATOM	4639	C	ALA	608	59.598	-1.979	26.352	1.00	28.94
ATOM	4640	O	ALA	608	59.889	-1.091	27.155	1.00	27.83
ATOM	4641	N	ARG	609	60.436	-2.959	26.032	1.00	28.79
ATOM	4643	CA	ARG	609	61.765	-3.023	26.628	1.00	30.90
ATOM	4644	CB	ARG	609	62.499	-4.291	26.206	1.00	35.84
ATOM	4645	CG	ARG	609	61.787	-5.571	26.527	1.00	41.94
ATOM	4646	CD	ARG	609	62.782	-6.707	26.575	1.00	44.70
ATOM	4647	NE	ARG	609	63.392	-6.821	27.900	1.00	47.13
ATOM	4649	CZ	ARG	609	64.444	-7.589	28.183	1.00	48.71
ATOM	4650	NH1	ARG	609	65.025	-8.314	27.233	1.00	48.33
ATOM	4653	NH2	ARG	609	64.897	-7.655	29.428	1.00	49.11
ATOM	4656	C	ARG	609	62.602	-1.815	26.207	1.00	32.38
ATOM	4657	O	ARG	609	63.215	-1.148	27.058	1.00	32.63
ATOM	4658	N	GLY	610	62.636	-1.554	24.894	1.00	29.98
ATOM	4660	CA	GLY	610	63.384	-0.430	24.358	1.00	25.65
ATOM	4661	C	GLY	610	62.969	0.837	25.061	1.00	25.44
ATOM	4662	O	GLY	610	63.791	1.640	25.463	1.00	27.09
ATOM	4663	N	MET	611	61.672	1.009	25.242	1.00	30.41
ATOM	4665	CA	MET	611	61.167	2.176	25.943	1.00	31.34
ATOM	4666	CB	MET	611	59.653	2.233	25.832	1.00	28.39
ATOM	4667	CG	MET	611	59.195	2.595	24.449	1.00	25.17
ATOM	4668	SD	MET	611	59.904	4.182	24.005	1.00	26.65
ATOM	4669	CE	MET	611	59.458	5.158	25.453	1.00	19.78
ATOM	4670	C	MET	611	61.600	2.176	27.412	1.00	34.05
ATOM	4671	O	MET	611	62.008	3.211	27.929	1.00	33.79
ATOM	4672	N	GLU	612	61.500	1.026	28.078	1.00	37.16
ATOM	4674	CA	GLU	612	61.893	0.913	29.484	1.00	38.85
ATOM	4675	CB	GLU	612	61.732	-0.533	29.988	1.00	38.96
ATOM	4676	CG	GLU	612	62.249	-0.788	31.400	1.00	35.19
ATOM	4677	CD	GLU	612	62.316	-2.271	31.783	1.00	35.26
ATOM	4678	OE1	GLU	612	62.605	-3.123	30.912	1.00	29.29

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ATOM	4679	OE2	GLU	612	62.102	-2.588	32.982	1.00	37.85
ATOM	4680	C	GLU	612	63.353	1.364	29.628	1.00	40.01
ATOM	4681	O	GLU	612	63.720	2.060	30.584	1.00	38.27
ATOM	4682	N	TYR	613	64.176	0.972	28.662	1.00	40.33
ATOM	4684	CA	TYR	613	65.575	1.362	28.664	1.00	39.71
ATOM	4685	CB	TYR	613	66.333	0.722	27.494	1.00	39.03
ATOM	4686	CG	TYR	613	67.800	1.100	27.467	1.00	41.41
ATOM	4687	CD1	TYR	613	68.702	0.527	28.364	1.00	42.79
ATOM	4688	CE1	TYR	613	70.048	0.905	28.386	1.00	40.21
ATOM	4689	CD2	TYR	613	68.283	2.068	26.581	1.00	39.75
ATOM	4690	CE2	TYR	613	69.621	2.454	26.596	1.00	39.01
ATOM	4691	CZ	TYR	613	70.499	1.868	27.503	1.00	39.56
ATOM	4692	OH	TYR	613	71.823	2.249	27.538	1.00	35.63
ATOM	4694	C	TYR	613	65.642	2.881	28.562	1.00	38.71
ATOM	4695	O	TYR	613	66.106	3.541	29.486	1.00	38.52
ATOM	4696	N	LEU	614	65.126	3.423	27.460	1.00	37.22
ATOM	4698	CA	LEU	614	65.128	4.864	27.212	1.00	35.66
ATOM	4699	CB	LEU	614	64.223	5.202	26.025	1.00	35.27
ATOM	4700	CG	LEU	614	64.687	4.699	24.659	1.00	33.09
ATOM	4701	CD1	LEU	614	63.718	5.188	23.612	1.00	33.31
ATOM	4702	CD2	LEU	614	66.099	5.184	24.363	1.00	31.20
ATOM	4703	C	LEU	614	64.672	5.653	28.430	1.00	35.64
ATOM	4704	O	LEU	614	65.298	6.639	28.816	1.00	34.54
ATOM	4705	N	ALA	615	63.577	5.203	29.032	1.00	36.61
ATOM	4707	CA	ALA	615	63.028	5.835	30.222	1.00	37.74
ATOM	4708	CB	ALA	615	61.682	5.187	30.608	1.00	37.74
ATOM	4709	C	ALA	615	64.021	5.776	31.389	1.00	37.30
ATOM	4710	O	ALA	615	64.111	6.731	32.175	1.00	37.29
ATOM	4711	N	SER	616	64.752	4.665	31.511	1.00	37.18
ATOM	4713	CA	SER	616	65.741	4.534	32.577	1.00	36.92
ATOM	4714	CB	SER	616	66.274	3.091	32.702	1.00	34.82
ATOM	4715	OG	SER	616	67.106	2.680	31.628	1.00	28.79
ATOM	4717	C	SER	616	66.870	5.516	32.287	1.00	38.57
ATOM	4718	O	SER	616	67.633	5.902	33.179	1.00	38.30
ATOM	4719	N	LYS	617	66.958	5.925	31.024	1.00	37.62
ATOM	4721	CA	LYS	617	67.965	6.876	30.606	1.00	36.13
ATOM	4722	CB	LYS	617	68.511	6.494	29.238	1.00	35.90
ATOM	4723	CG	LYS	617	69.274	5.206	29.236	1.00	34.58
ATOM	4724	CD	LYS	617	70.502	5.348	30.077	1.00	35.44
ATOM	4725	CE	LYS	617	71.201	4.022	30.232	1.00	38.54
ATOM	4726	NZ	LYS	617	72.566	4.211	30.790	1.00	41.54
ATOM	4730	C	LYS	617	67.378	8.275	30.564	1.00	36.55
ATOM	4731	O	LYS	617	67.943	9.155	29.934	1.00	40.26
ATOM	4732	N	LYS	618	66.221	8.468	31.187	1.00	36.42
ATOM	4734	CA	LYS	618	65.570	9.779	31.231	1.00	36.06
ATOM	4735	CB	LYS	618	66.543	10.833	31.746	1.00	42.22
ATOM	4736	CG	LYS	618	67.234	10.499	33.062	1.00	52.36
ATOM	4737	CD	LYS	618	66.301	10.668	34.236	1.00	61.51
ATOM	4738	CE	LYS	618	66.933	10.121	35.495	1.00	67.28
ATOM	4739	NZ	LYS	618	65.965	10.161	36.618	1.00	73.99
ATOM	4743	C	LYS	618	65.026	10.261	29.887	1.00	34.94
ATOM	4744	O	LYS	618	64.562	11.393	29.781	1.00	34.69

ATOM	4745	N	CYS	619	65.051	9.407	28.872	1.00	34.46
ATOM	4747	CA	CYS	619	64.588	9.793	27.543	1.00	33.12
ATOM	4748	CB	CYS	619	65.311	8.966	26.475	1.00	34.33
ATOM	4749	SG	CYS	619	64.920	9.397	24.778	1.00	35.64
ATOM	4750	C	CYS	619	63.075	9.699	27.355	1.00	32.13
ATOM	4751	O	CYS	619	62.465	8.645	27.584	1.00	30.72
ATOM	4752	N	ILE	620	62.477	10.818	26.960	1.00	32.70
ATOM	4754	CA	ILE	620	61.046	10.909	26.708	1.00	32.75
ATOM	4755	CB	ILE	620	60.440	12.129	27.421	1.00	33.55
ATOM	4756	CG2	ILE	620	59.002	12.339	26.986	1.00	38.39
ATOM	4757	CG1	ILE	620	60.486	11.913	28.933	1.00	30.71
ATOM	4758	CD1	ILE	620	59.994	13.084	29.710	1.00	30.11
ATOM	4759	C	ILE	620	60.969	11.086	25.206	1.00	33.31
ATOM	4760	O	ILE	620	61.516	12.040	24.674	1.00	33.40
ATOM	4761	N	HIS	621	60.356	10.114	24.533	1.00	33.56
ATOM	4763	CA	HIS	621	60.230	10.092	23.087	1.00	32.30
ATOM	4764	CB	HIS	621	59.866	8.668	22.642	1.00	29.55
ATOM	4765	CG	HIS	621	60.049	8.402	21.173	1.00	27.32
ATOM	4766	CD2	HIS	621	60.694	7.404	20.533	1.00	24.26
ATOM	4767	ND1	HIS	621	59.462	9.173	20.187	1.00	25.20
ATOM	4769	CE1	HIS	621	59.734	8.652	19.006	1.00	25.81
ATOM	4770	NE2	HIS	621	60.481	7.579	19.184	1.00	26.65
ATOM	4772	C	HIS	621	59.246	11.103	22.499	1.00	35.40
ATOM	4773	O	HIS	621	59.459	11.574	21.388	1.00	39.18
ATOM	4774	N	ARG	622	58.128	11.363	23.178	1.00	36.39
ATOM	4776	CA	ARG	622	57.117	12.323	22.686	1.00	36.40
ATOM	4777	CB	ARG	622	57.694	13.732	22.617	1.00	35.62
ATOM	4778	CG	ARG	622	58.171	14.253	23.937	1.00	33.79
ATOM	4779	CD	ARG	622	58.837	15.591	23.759	0.50	32.17
ATOM	4780	NE	ARG	622	59.315	16.101	25.032	0.50	32.82
ATOM	4782	CZ	ARG	622	60.487	15.786	25.575	0.50	34.07
ATOM	4783	NH1	ARG	622	61.326	14.965	24.952	0.50	33.44
ATOM	4786	NH2	ARG	622	60.803	16.268	26.769	0.50	32.70
ATOM	4789	C	ARG	622	56.405	12.008	21.355	1.00	36.23
ATOM	4790	O	ARG	622	55.527	12.763	20.936	1.00	35.04
ATOM	4791	N	ASP	623	56.806	10.938	20.668	1.00	35.84
ATOM	4793	CA	ASP	623	56.128	10.538	19.436	1.00	35.68
ATOM	4794	CB	ASP	623	56.574	11.352	18.221	1.00	38.71
ATOM	4795	CG	ASP	623	55.736	11.036	16.974	1.00	46.29
ATOM	4796	OD1	ASP	623	56.277	11.082	15.851	1.00	52.33
ATOM	4797	OD2	ASP	623	54.535	10.715	17.119	1.00	50.45
ATOM	4798	C	ASP	623	56.271	9.052	19.162	1.00	32.98
ATOM	4799	O	ASP	623	56.664	8.645	18.073	1.00	30.90
ATOM	4800	N	LEU	624	56.015	8.244	20.179	1.00	31.16
ATOM	4802	CA	LEU	624	56.099	6.801	20.029	1.00	31.71
ATOM	4803	CB	LEU	624	56.070	6.144	21.407	1.00	28.48
ATOM	4804	CG	LEU	624	56.049	4.618	21.514	1.00	28.13
ATOM	4805	CD1	LEU	624	57.225	3.975	20.799	1.00	27.00
ATOM	4806	CD2	LEU	624	56.072	4.283	22.987	1.00	29.10
ATOM	4807	C	LEU	624	54.917	6.320	19.185	1.00	32.67
ATOM	4808	O	LEU	624	53.763	6.608	19.508	1.00	35.74
ATOM	4809	N	ALA	625	55.214	5.640	18.081	1.00	29.82

ATOM	4811	CA	ALA	625	54.194	5.106	17.181	1.00	28.29
ATOM	4812	CB	ALA	625	53.682	6.182	16.245	1.00	26.72
ATOM	4813	C	ALA	625	54.895	4.031	16.395	1.00	28.40
ATOM	4814	O	ALA	625	56.118	4.028	16.343	1.00	32.12
ATOM	4815	N	ALA	626	54.131	3.135	15.770	1.00	28.55
ATOM	4817	CA	ALA	626	54.687	2.028	14.979	1.00	26.25
ATOM	4818	CB	ALA	626	53.577	1.169	14.365	1.00	23.54
ATOM	4819	C	ALA	626	55.569	2.573	13.892	1.00	23.68
ATOM	4820	O	ALA	626	56.544	1.944	13.519	1.00	26.07
ATOM	4821	N	ARG	627	55.208	3.744	13.378	1.00	23.80
ATOM	4823	CA	ARG	627	55.980	4.413	12.338	1.00	26.57
ATOM	4824	CB	ARG	627	55.289	5.728	11.914	1.00	25.91
ATOM	4825	CG	ARG	627	54.991	6.692	13.055	1.00	27.60
ATOM	4826	CD	ARG	627	54.711	8.130	12.584	1.00	33.01
ATOM	4827	NE	ARG	627	54.260	8.978	13.691	1.00	34.18
ATOM	4829	CZ	ARG	627	52.997	9.067	14.091	1.00	35.88
ATOM	4830	NH1	ARG	627	52.056	8.380	13.460	1.00	38.89
ATOM	4833	NH2	ARG	627	52.689	9.748	15.183	1.00	36.43
ATOM	4836	C	ARG	627	57.439	4.686	12.785	1.00	29.03
ATOM	4837	O	ARG	627	58.362	4.606	11.972	1.00	29.24
ATOM	4838	N	ASN	628	57.634	4.938	14.087	1.00	29.51
ATOM	4840	CA	ASN	628	58.954	5.234	14.645	1.00	26.41
ATOM	4841	CB	ASN	628	58.864	6.359	15.676	1.00	25.32
ATOM	4842	CG	ASN	628	58.539	7.687	15.035	1.00	28.11
ATOM	4843	OD1	ASN	628	59.079	8.028	13.999	1.00	32.09
ATOM	4844	ND2	ASN	628	57.639	8.426	15.628	1.00	27.88
ATOM	4847	C	ASN	628	59.684	4.039	15.225	1.00	25.77
ATOM	4848	O	ASN	628	60.641	4.188	16.001	1.00	24.77
ATOM	4849	N	VAL	629	59.209	3.853	14.874	1.00	26.63
ATOM	4851	CA	VAL	629	59.828	1.610	15.315	1.00	25.34
ATOM	4852	CB	VAL	629	58.812	0.693	16.007	1.00	21.26
ATOM	4853	CG1	VAL	629	59.492	-0.604	16.412	1.00	22.96
ATOM	4854	CG2	VAL	629	58.205	1.398	17.207	1.00	16.65
ATOM	4855	C	VAL	629	60.266	0.962	14.007	1.00	26.79
ATOM	4856	O	VAL	629	59.454	0.839	13.087	1.00	28.60
ATOM	4857	N	LEU	630	61.542	0.603	13.904	1.00	25.91
ATOM	4859	CA	LEU	630	62.062	-0.021	12.685	1.00	26.95
ATOM	4860	CB	LEU	630	63.297	0.733	12.210	1.00	22.79
ATOM	4861	CG	LEU	630	63.044	2.242	12.111	1.00	20.04
ATOM	4862	CD1	LEU	630	64.345	2.944	11.972	1.00	11.86
ATOM	4863	CD2	LEU	630	62.111	2.603	10.965	1.00	19.22
ATOM	4864	C	LEU	630	62.367	-1.492	12.961	1.00	28.01
ATOM	4865	O	LEU	630	62.629	-1.852	14.101	1.00	28.26
ATOM	4866	N	VAL	631	62.246	-2.346	11.946	1.00	30.82
ATOM	4868	CA	VAL	631	62.468	-3.790	12.098	1.00	31.75
ATOM	4869	CB	VAL	631	61.194	-4.607	11.659	1.00	30.04
ATOM	4870	CG1	VAL	631	61.346	-6.085	12.026	1.00	29.25
ATOM	4871	CG2	VAL	631	59.937	-4.030	12.290	1.00	24.59
ATOM	4872	C	VAL	631	63.697	-4.286	11.305	1.00	35.24
ATOM	4873	O	VAL	631	63.849	-3.999	10.097	1.00	34.02
ATOM	4874	N	THR	632	64.551	-5.052	11.979	1.00	36.24
ATOM	4876	CA	THR	632	65.770	-5.574	11.365	1.00	38.23

ATOM	4877	CB	THR	632	66.843	-5.836	12.416	1.00	38.21
ATOM	4878	OG1	THR	632	66.423	-6.908	13.272	1.00	38.31
ATOM	4880	CG2	THR	632	67.069	-4.582	13.238	1.00	40.22
ATOM	4881	C	THR	632	65.526	-6.854	10.593	1.00	39.17
ATOM	4882	O	THR	632	64.471	-7.457	10.744	1.00	41.26
ATOM	4883	N	GLU	633	66.496	-7.259	9.766	1.00	41.23
ATOM	4885	CA	GLU	633	66.397	-8.483	8.960	1.00	42.62
ATOM	4886	CB	GLU	633	67.677	-8.712	8.154	1.00	44.25
ATOM	4887	CG	GLU	633	67.610	-9.884	7.154	1.00	51.05
ATOM	4888	CD	GLU	633	66.825	-9.594	5.858	1.00	56.28
ATOM	4889	OE1	GLU	633	66.390	-8.444	5.626	1.00	62.64
ATOM	4890	OE2	GLU	633	66.651	-10.536	5.058	1.00	58.41
ATOM	4891	C	GLU	633	66.097	-9.722	9.797	1.00	41.93
ATOM	4892	O	GLU	633	65.578	-10.704	9.288	1.00	42.77
ATOM	4893	N	ASP	634	66.415	-9.665	11.082	1.00	43.14
ATOM	4895	CA	ASP	634	66.167	-10.784	11.978	1.00	44.01
ATOM	4896	CB	ASP	634	67.361	-11.007	12.914	1.00	49.37
ATOM	4897	CG	ASP	634	68.636	-11.396	12.166	1.00	54.70
ATOM	4898	OD1	ASP	634	68.683	-12.515	11.595	1.00	55.43
ATOM	4899	OD2	ASP	634	69.602	-10.596	12.167	1.00	56.17
ATOM	4900	C	ASP	634	64.925	-10.507	12.801	1.00	43.95
ATOM	4901	O	ASP	634	64.754	-11.085	13.864	1.00	45.92
ATOM	4902	N	ASN	635	64.075	-9.604	12.316	1.00	44.71
ATOM	4904	CA	ASN	635	62.822	-9.220	12.980	1.00	43.07
ATOM	4905	CB	ASN	635	61.854	-10.404	13.018	1.00	45.50
ATOM	4906	CG	ASN	635	61.606	-10.994	11.653	1.00	45.43
ATOM	4907	OD1	ASN	635	60.997	-10.369	10.788	1.00	49.56
ATOM	4908	ND2	ASN	635	62.114	-12.190	11.435	1.00	48.18
ATOM	4911	C	ASN	635	62.927	-8.609	14.380	1.00	41.64
ATOM	4912	O	ASN	635	62.050	-8.814	15.221	1.00	41.69
ATOM	4913	N	VAL	636	63.984	-7.843	14.627	1.00	41.17
ATOM	4915	CA	VAL	636	64.177	-7.178	15.922	1.00	39.01
ATOM	4916	CB	VAL	636	65.692	-7.002	16.259	1.00	40.66
ATOM	4917	CG1	VAL	636	65.882	-6.209	17.560	1.00	35.04
ATOM	4918	CG2	VAL	636	66.355	-8.360	16.367	1.00	41.69
ATOM	4919	C	VAL	636	63.544	-5.789	15.925	1.00	36.77
ATOM	4920	O	VAL	636	63.817	-4.989	15.045	1.00	38.35
ATOM	4921	N	MET	637	62.696	-5.518	16.908	1.00	35.71
ATOM	4923	CA	MET	637	62.049	-4.216	17.031	1.00	33.65
ATOM	4924	CB	MET	637	60.783	-4.319	17.884	1.00	38.24
ATOM	4925	CG	MET	637	59.737	-5.314	17.371	1.00	41.34
ATOM	4926	SD	MET	637	59.128	-4.993	15.695	1.00	42.24
ATOM	4927	CE	MET	637	59.249	-6.621	14.976	1.00	39.27
ATOM	4928	C	MET	637	63.001	-3.209	17.668	1.00	32.62
ATOM	4929	O	MET	637	63.524	-3.436	18.765	1.00	30.56
ATOM	4930	N	LYS	638	63.173	-2.070	17.008	1.00	32.03
ATOM	4932	CA	LYS	638	64.073	-1.027	17.492	1.00	28.77
ATOM	4933	CB	LYS	638	65.351	-1.022	16.654	1.00	27.71
ATOM	4934	CG	LYS	638	66.245	-2.211	16.896	1.00	25.04
ATOM	4935	CD	LYS	638	67.429	-2.170	15.976	1.00	24.50
ATOM	4936	CE	LYS	638	68.443	-3.187	16.390	1.00	22.85
ATOM	4937	NZ	LYS	638	69.121	-2.803	17.651	1.00	24.79

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ATOM	4941	C	LYS	638	63.443	0.364	17.446	1.00	28.00
ATOM	4942	O	LYS	638	62.977	0.799	16.391	1.00	25.60
ATOM	4943	N	ILE	639	63.410	1.032	18.601	1.00	25.32
ATOM	4945	CA	ILE	639	62.857	2.379	18.721	1.00	25.91
ATOM	4946	CB	ILE	639	62.800	2.875	20.201	1.00	25.56
ATOM	4947	CG2	ILE	639	62.074	4.208	20.279	1.00	22.82
ATOM	4948	CG1	ILE	639	62.142	1.835	21.118	1.00	28.00
ATOM	4949	CD1	ILE	639	60.634	1.748	21.003	1.00	33.25
ATOM	4950	C	ILE	639	63.739	3.363	17.955	1.00	26.87
ATOM	4951	O	ILE	639	64.968	3.381	18.125	1.00	24.13
ATOM	4952	N	ALA	640	63.108	4.170	17.108	1.00	26.74
ATOM	4954	CA	ALA	640	63.825	5.176	16.339	1.00	30.62
ATOM	4955	CB	ALA	640	63.624	4.939	14.851	1.00	30.31
ATOM	4956	C	ALA	640	63.338	6.572	16.739	1.00	32.53
ATOM	4957	O	ALA	640	62.289	6.706	17.371	1.00	33.83
ATOM	4958	N	ASP	641	64.082	7.605	16.351	1.00	33.05
ATOM	4960	CA	ASP	641	63.749	9.010	16.656	1.00	37.66
ATOM	4961	CB	ASP	641	62.539	9.483	15.840	1.00	42.62
ATOM	4962	CG	ASP	641	62.928	10.026	14.471	1.00	50.92
ATOM	4963	OD1	ASP	641	64.092	9.833	14.021	1.00	59.21
ATOM	4964	OD2	ASP	641	62.063	10.652	13.823	1.00	54.05
ATOM	4965	C	ASP	641	63.545	9.367	18.125	1.00	37.85
ATOM	4966	O	ASP	641	62.805	10.294	18.448	1.00	39.10
ATOM	4967	N	PHE	642	64.204	8.635	19.016	1.00	37.47
ATOM	4969	CA	PHE	642	64.099	8.874	20.456	1.00	36.47
ATOM	4970	CB	PHE	642	64.403	7.581	21.226	1.00	32.22
ATOM	4971	CG	PHE	642	65.786	7.013	20.964	1.00	30.65
ATOM	4972	CD1	PHE	642	66.906	7.537	21.607	1.00	32.45
ATOM	4973	CD2	PHE	642	65.969	5.981	20.054	1.00	28.53
ATOM	4974	CE1	PHE	642	68.180	7.050	21.342	1.00	30.88
ATOM	4975	CE2	PHE	642	67.234	5.494	19.789	1.00	27.74
ATOM	4976	CZ	PHE	642	68.344	6.027	20.431	1.00	29.64
ATOM	4977	C	PHE	642	65.050	10.001	20.907	1.00	39.69
ATOM	4978	O	PHE	642	64.967	10.469	22.047	1.00	38.22
ATOM	4979	N	GLY	643	65.966	10.400	20.015	1.00	41.08
ATOM	4981	CA	GLY	643	66.925	11.447	20.324	1.00	40.65
ATOM	4982	C	GLY	643	66.694	12.747	19.571	1.00	43.53
ATOM	4983	O	GLY	643	67.500	13.666	19.688	1.00	41.10
ATOM	4984	N	LEU	644	65.617	12.825	18.786	1.00	48.35
ATOM	4986	CA	LEU	644	65.306	14.034	18.019	1.00	51.11
ATOM	4987	CB	LEU	644	63.962	13.907	17.314	1.00	50.28
ATOM	4988	CG	LEU	644	63.900	13.059	16.057	1.00	54.03
ATOM	4989	CD1	LEU	644	62.541	13.278	15.413	1.00	57.34
ATOM	4990	CD2	LEU	644	65.006	13.467	15.105	1.00	56.95
ATOM	4991	C	LEU	644	65.248	15.257	18.894	1.00	52.68
ATOM	4992	O	LEU	644	64.850	15.175	20.053	1.00	54.95
ATOM	4993	N	ALA	645	65.629	16.399	18.332	1.00	54.61
ATOM	4995	CA	ALA	645	65.610	17.656	19.073	1.00	54.60
ATOM	4996	CB	ALA	645	66.495	18.684	18.382	1.00	53.32
ATOM	4997	C	ALA	645	64.178	18.185	19.215	1.00	54.09
ATOM	4998	O	ALA	645	63.716	18.488	20.322	1.00	53.14
ATOM	4999	N	ASP	652	52.340	21.795	14.895	1.00	91.33

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ATOM	5001	CA	ASP	652	51.194	21.914	14.004	1.00	90.97
ATOM	5002	CB	ASP	652	51.650	22.138	12.555	1.00	92.06
ATOM	5003	CG	ASP	652	50.488	22.434	11.606	1.00	94.00
ATOM	5004	OD1	ASP	652	49.479	23.032	12.042	1.00	95.25
ATOM	5005	OD2	ASP	652	50.586	22.075	10.414	1.00	94.81
ATOM	5006	C	ASP	652	50.352	20.652	14.103	1.00	90.61
ATOM	5007	O	ASP	652	50.645	19.641	13.463	1.00	91.26
ATOM	5008	N	TYR	653	49.289	20.737	14.895	1.00	89.65
ATOM	5010	CA	TYR	653	48.381	19.619	15.110	1.00	88.25
ATOM	5011	CB	TYR	653	47.306	20.003	16.133	1.00	88.16
ATOM	5012	CG	TYR	653	47.800	20.140	17.559	1.00	88.74
ATOM	5013	CD1	TYR	653	47.047	20.818	18.513	1.00	90.00
ATOM	5014	CE1	TYR	653	47.477	20.915	19.839	1.00	90.70
ATOM	5015	CD2	TYR	653	49.006	19.559	17.964	1.00	89.14
ATOM	5016	CE2	TYR	653	49.443	19.649	19.280	1.00	89.49
ATOM	5017	CZ	TYR	653	48.675	20.325	20.214	1.00	89.80
ATOM	5018	OH	TYR	653	49.109	20.394	21.518	1.00	89.81
ATOM	5020	C	TYR	653	47.701	19.165	13.830	1.00	87.32
ATOM	5021	O	TYR	653	47.180	18.057	13.759	1.00	87.70
ATOM	5022	N	TYR	654	47.734	20.013	12.814	1.00	86.51
ATOM	5024	CA	TYR	654	47.087	19.707	11.553	1.00	87.08
ATOM	5025	CB	TYR	654	46.387	20.959	11.028	1.00	88.45
ATOM	5026	CG	TYR	654	45.375	21.497	12.014	1.00	90.25
ATOM	5027	CD1	TYR	654	45.781	22.017	13.246	1.00	90.15
ATOM	5028	CE1	TYR	654	44.857	22.431	14.197	1.00	90.94
ATOM	5029	CD2	TYR	654	44.012	21.419	11.753	1.00	91.22
ATOM	5030	CE2	TYR	654	43.078	21.833	12.698	1.00	93.22
ATOM	5031	CZ	TYR	654	43.506	22.335	13.918	1.00	92.39
ATOM	5032	OH	TYR	654	42.588	22.717	14.872	1.00	94.38
ATOM	5034	C	TYR	654	48.012	19.115	10.503	1.00	87.34
ATOM	5035	O	TYR	654	47.567	18.767	9.410	1.00	88.29
ATOM	5036	N	LYS	655	49.290	18.971	10.836	1.00	86.67
ATOM	5038	CA	LYS	655	50.233	18.406	9.987	1.00	87.62
ATOM	5039	CB	LYS	655	51.666	18.814	10.229	1.00	90.01
ATOM	5040	CG	LYS	655	52.688	18.252	9.251	1.00	95.23
ATOM	5041	CD	LYS	655	54.106	18.646	9.607	1.00	99.04
ATOM	5042	CE	LYS	655	55.108	17.832	8.789	1.00	102.26
ATOM	5043	NZ	LYS	655	56.528	18.184	9.099	1.00	104.44
ATOM	5047	C	LYS	655	50.102	16.890	9.896	1.00	87.61
ATOM	5048	O	LYS	655	50.233	16.259	10.945	1.00	87.58
ATOM	5049	N	LYS	656	49.787	16.319	8.737	1.00	87.88
ATOM	5051	CA	LYS	656	49.639	14.875	8.603	1.00	89.03
ATOM	5052	CB	LYS	656	48.795	14.537	7.376	1.00	90.44
ATOM	5053	CG	LYS	656	47.313	14.802	7.535	1.00	93.30
ATOM	5054	CD	LYS	656	46.590	14.599	6.213	1.00	96.87
ATOM	5055	CE	LYS	656	45.089	14.555	6.406	1.00	99.35
ATOM	5056	NZ	LYS	656	44.362	14.518	5.106	1.00	102.42
ATOM	5060	C	LYS	656	51.004	14.206	8.487	1.00	88.57
ATOM	5061	O	LYS	656	51.915	14.749	7.855	1.00	88.38
ATOM	5062	N	GLY	660	49.270	10.021	5.735	1.00	61.58
ATOM	5064	CA	GLY	660	48.416	11.168	6.005	1.00	58.75
ATOM	5065	C	GLY	660	47.664	11.092	7.324	1.00	57.22

ATOM	5066	O	GLY	660	46.555	11.624	7.437	1.00	58.01
ATOM	5067	N	ARG	661	48.231	10.374	8.293	1.00	55.37
ATOM	5069	CA	ARG	661	47.631	10.247	9.622	1.00	51.19
ATOM	5070	CB	ARG	661	48.095	8.965	10.337	1.00	51.89
ATOM	5071	CG	ARG	661	47.756	7.663	9.612	1.00	51.56
ATOM	5072	CD	ARG	661	48.057	6.443	10.484	1.00	50.77
ATOM	5073	NE	ARG	661	47.834	5.181	9.772	1.00	50.04
ATOM	5075	CZ	ARG	661	48.015	3.974	10.307	1.00	48.12
ATOM	5076	NH1	ARG	661	48.421	3.855	11.569	1.00	43.28
ATOM	5079	NH2	ARG	661	47.788	2.882	9.578	1.00	43.69
ATOM	5082	C	ARG	661	48.041	11.463	10.446	1.00	46.22
ATOM	5083	O	ARG	661	48.998	12.162	10.097	1.00	44.78
ATOM	5084	N	LEU	662	47.328	11.703	11.542	1.00	41.80
ATOM	5086	CA	LEU	662	47.621	12.837	12.419	1.00	36.78
ATOM	5087	CB	LEU	662	46.342	13.596	12.758	1.00	33.05
ATOM	5088	CG	LEU	662	45.642	14.279	11.585	1.00	28.24
ATOM	5089	CD1	LEU	662	44.198	14.611	11.935	1.00	24.66
ATOM	5090	CD2	LEU	662	46.429	15.511	11.217	1.00	28.35
ATOM	5091	C	LEU	662	48.278	12.328	13.695	1.00	36.10
ATOM	5092	O	LEU	662	47.695	11.521	14.431	1.00	34.46
ATOM	5093	N	PRO	663	49.526	12.751	13.945	1.00	35.83
ATOM	5094	CD	PRO	663	50.360	13.537	13.022	1.00	37.72
ATOM	5095	CA	PRO	663	50.310	12.365	15.119	1.00	35.68
ATOM	5096	CB	PRO	663	51.611	13.130	14.914	1.00	35.23
ATOM	5097	CG	PRO	663	51.756	13.134	13.437	1.00	36.10
ATOM	5098	C	PRO	663	49.660	12.703	16.453	1.00	35.87
ATOM	5099	O	PRO	663	49.958	12.069	17.469	1.00	39.86
ATOM	5100	N	VAL	664	48.787	13.705	16.466	1.00	33.54
ATOM	5102	CA	VAL	664	48.109	14.076	17.699	1.00	31.24
ATOM	5103	CB	VAL	664	47.196	15.321	17.520	1.00	30.45
ATOM	5104	CG1	VAL	664	48.025	16.480	17.051	1.00	32.54
ATOM	5105	CG2	VAL	664	46.093	15.062	16.523	1.00	34.77
ATOM	5106	C	VAL	664	47.301	12.895	18.233	1.00	31.33
ATOM	5107	O	VAL	664	47.095	12.782	19.438	1.00	32.66
ATOM	5108	N	LYS	665	46.940	11.968	17.345	1.00	30.44
ATOM	5110	CA	LYS	665	46.153	10.795	17.719	1.00	28.43
ATOM	5111	CB	LYS	665	45.596	10.133	16.466	1.00	24.82
ATOM	5112	CG	LYS	665	44.700	11.080	15.687	1.00	27.50
ATOM	5113	CD	LYS	665	44.096	10.466	14.442	1.00	26.62
ATOM	5114	CE	LYS	665	42.967	11.326	13.909	1.00	21.64
ATOM	5115	NZ	LYS	665	42.479	10.850	12.584	1.00	25.29
ATOM	5119	C	LYS	665	46.889	9.794	18.615	1.00	29.56
ATOM	5120	O	LYS	665	46.295	8.836	19.095	1.00	29.57
ATOM	5121	N	TRP	666	48.183	10.020	18.826	1.00	30.12
ATOM	5123	CA	TRP	666	48.987	9.174	19.704	1.00	31.39
ATOM	5124	CB	TRP	666	50.329	8.845	19.059	1.00	30.40
ATOM	5125	CG	TRP	666	50.263	7.700	18.106	1.00	30.79
ATOM	5126	CD2	TRP	666	49.701	7.719	16.785	1.00	30.22
ATOM	5127	CE2	TRP	666	49.891	6.430	16.245	1.00	28.24
ATOM	5128	CE3	TRP	666	49.067	8.702	16.012	1.00	30.60
ATOM	5129	CD1	TRP	666	50.743	6.435	18.307	1.00	28.07
ATOM	5130	NE1	TRP	666	50.522	5.670	17.187	1.00	29.15

ATOM	5132	CZ2	TRP	666	49.462	6.107	14.954	1.00	29.38
ATOM	5133	CZ3	TRP	666	48.640	8.374	14.726	1.00	31.27
ATOM	5134	CH2	TRP	666	48.845	7.086	14.213	1.00	31.33
ATOM	5135	C	TRP	666	49.242	9.902	21.026	1.00	33.92
ATOM	5136	O	TRP	666	49.591	9.287	22.040	1.00	35.23
ATOM	5137	N	MET	667	49.028	11.214	21.007	1.00	35.72
ATOM	5139	CA	MET	667	49.260	12.065	22.159	1.00	36.43
ATOM	5140	CB	MET	667	49.163	13.529	21.751	1.00	37.70
ATOM	5141	CG	MET	667	50.510	14.194	21.574	1.00	40.10
ATOM	5142	SD	MET	667	50.358	15.906	21.096	1.00	46.91
ATOM	5143	CE	MET	667	50.914	15.810	19.386	1.00	40.40
ATOM	5144	C	MET	667	48.389	11.839	23.378	1.00	38.36
ATOM	5145	O	MET	667	47.186	11.646	23.273	1.00	39.53
ATOM	5146	N	ALA	668	49.027	11.885	24.542	1.00	39.93
ATOM	5148	CA	ALA	668	48.345	11.733	25.815	1.00	38.48
ATOM	5149	CB	ALA	668	49.351	11.537	26.929	1.00	37.61
ATOM	5150	C	ALA	668	47.603	13.038	26.014	1.00	39.48
ATOM	5151	O	ALA	668	48.059	14.090	25.566	1.00	39.40
ATOM	5152	N	PRO	669	46.474	13.001	26.731	1.00	42.22
ATOM	5153	CD	PRO	669	45.842	11.827	27.355	1.00	42.77
ATOM	5154	CA	PRO	669	45.677	14.204	26.980	1.00	43.91
ATOM	5155	CB	PRO	669	44.609	13.698	27.948	1.00	44.49
ATOM	5156	CG	PRO	669	44.421	12.279	27.499	1.00	43.59
ATOM	5157	C	PRO	669	46.476	15.372	27.570	1.00	44.89
ATOM	5158	O	PRO	669	46.394	16.497	27.075	1.00	45.48
ATOM	5159	N	GLU	670	47.266	15.105	28.607	1.00	43.39
ATOM	5161	CA	GLU	670	48.050	16.158	29.244	1.00	42.97
ATOM	5162	CB	GLU	670	48.739	15.645	30.504	1.00	43.31
ATOM	5163	CG	GLU	670	49.864	14.646	30.252	1.00	44.78
ATOM	5164	CD	GLU	670	49.408	13.204	30.290	1.00	43.48
ATOM	5165	OE1	GLU	670	50.225	12.331	30.639	1.00	41.85
ATOM	5166	OE2	GLU	670	48.235	12.931	29.986	1.00	47.18
ATOM	5167	C	GLU	670	49.090	16.798	28.333	1.00	43.18
ATOM	5168	O	GLU	670	49.362	17.983	28.444	1.00	41.68
ATOM	5169	N	ALA	671	49.677	16.008	27.440	1.00	44.65
ATOM	5171	CA	ALA	671	50.686	16.512	26.513	1.00	44.44
ATOM	5172	CB	ALA	671	51.412	15.347	25.841	1.00	40.17
ATOM	5173	C	ALA	671	50.046	17.410	25.465	1.00	46.49
ATOM	5174	O	ALA	671	50.558	18.484	25.148	1.00	45.70
ATOM	5175	N	LEU	672	48.903	16.970	24.952	1.00	50.30
ATOM	5177	CA	LEU	672	48.163	17.702	23.925	1.00	52.07
ATOM	5178	CB	LEU	672	47.080	16.782	23.335	1.00	54.41
ATOM	5179	CG	LEU	672	46.388	17.103	22.005	1.00	57.12
ATOM	5180	CD1	LEU	672	47.404	17.316	20.912	1.00	57.65
ATOM	5181	CD2	LEU	672	45.459	15.951	21.640	1.00	56.14
ATOM	5182	C	LEU	672	47.535	18.964	24.512	1.00	52.42
ATOM	5183	O	LEU	672	47.683	20.058	23.969	1.00	52.71
ATOM	5184	N	PHE	673	46.863	18.803	25.645	1.00	52.74
ATOM	5186	CA	PHE	673	46.203	19.911	26.314	1.00	54.32
ATOM	5187	CB	PHE	673	44.995	19.394	27.104	1.00	52.92
ATOM	5188	CG	PHE	673	43.987	18.646	26.259	1.00	52.38
ATOM	5189	CD1	PHE	673	43.399	17.477	26.728	1.00	53.49

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ATOM	5190	CD2	PHE	673	43.624	19.109	24.999	1.00	51.61
ATOM	5191	CE1	PHE	673	42.468	16.779	25.957	1.00	50.49
ATOM	5192	CE2	PHE	673	42.698	18.420	24.229	1.00	50.91
ATOM	5193	CZ	PHE	673	42.118	17.250	24.710	1.00	50.09
ATOM	5194	C	PHE	673	47.138	20.732	27.220	1.00	56.29
ATOM	5195	O	PHE	673	47.289	21.938	27.026	1.00	58.05
ATOM	5196	N	ASP	674	47.808	20.076	28.165	1.00	56.38
ATOM	5198	CA	ASP	674	48.703	20.772	29.104	1.00	56.12
ATOM	5199	CB	ASP	674	48.644	20.101	30.485	1.00	53.81
ATOM	5200	CG	ASP	674	47.299	20.234	31.152	1.00	52.48
ATOM	5201	OD1	ASP	674	46.715	19.188	31.504	1.00	50.25
ATOM	5202	OD2	ASP	674	46.844	21.384	31.337	1.00	51.16
ATOM	5203	C	ASP	674	50.182	20.886	28.706	1.00	57.07
ATOM	5204	O	ASP	674	51.010	21.273	29.541	1.00	56.00
ATOM	5205	N	ARG	675	50.525	20.526	27.468	1.00	57.28
ATOM	5207	CA	ARG	675	51.915	20.576	26.995	1.00	55.64
ATOM	5208	CB	ARG	675	52.341	22.020	26.692	1.00	58.95
ATOM	5209	CG	ARG	675	51.542	22.678	25.569	1.00	66.91
ATOM	5210	CD	ARG	675	52.082	24.066	25.202	1.00	72.90
ATOM	5211	NE	ARG	675	53.360	24.019	24.482	1.00	75.10
ATOM	5213	CZ	ARG	675	54.096	25.089	24.181	1.00	73.61
ATOM	5214	NH1	ARG	675	53.687	26.301	24.536	1.00	71.27
ATOM	5217	NH2	ARG	675	55.250	24.943	23.540	1.00	72.12
ATOM	5220	C	ARG	675	52.853	19.932	28.017	1.00	53.25
ATOM	5221	O	ARG	675	53.988	20.366	28.211	1.00	52.13
ATOM	5222	N	ILE	676	52.359	18.883	28.664	1.00	51.44
ATOM	5224	CA	ILE	676	53.108	18.153	29.683	1.00	49.81
ATOM	5225	CB	ILE	676	52.241	17.944	30.958	1.00	46.07
ATOM	5226	CG2	ILE	676	52.804	16.844	31.856	1.00	40.98
ATOM	5227	CG1	ILE	676	52.129	19.257	31.721	1.00	43.31
ATOM	5228	CD1	ILE	676	51.324	19.147	32.963	1.00	45.02
ATOM	5229	C	ILE	676	53.572	16.800	29.144	1.00	51.20
ATOM	5230	O	ILE	676	52.770	15.892	28.951	1.00	52.37
ATOM	5231	N	TYR	677	54.865	16.675	28.890	1.00	52.81
ATOM	5233	CA	TYR	677	55.412	15.429	28.383	1.00	53.96
ATOM	5234	CB	TYR	677	56.296	15.700	27.167	1.00	57.26
ATOM	5235	CG	TYR	677	55.524	16.175	25.951	1.00	64.10
ATOM	5236	CD1	TYR	677	55.229	17.532	25.762	1.00	65.60
ATOM	5237	CE1	TYR	677	54.514	17.965	24.634	1.00	67.15
ATOM	5238	CD2	TYR	677	55.085	15.263	24.985	1.00	66.29
ATOM	5239	CE2	TYR	677	54.376	15.680	23.862	1.00	67.34
ATOM	5240	CZ	TYR	677	54.095	17.028	23.692	1.00	69.24
ATOM	5241	OH	TYR	677	53.399	17.414	22.573	1.00	73.55
ATOM	5243	C	TYR	677	56.192	14.713	29.482	1.00	52.30
ATOM	5244	O	TYR	677	57.053	15.309	30.124	1.00	53.73
ATOM	5245	N	THR	678	55.830	13.461	29.748	1.00	48.95
ATOM	5247	CA	THR	678	56.505	12.659	30.760	1.00	45.99
ATOM	5248	CB	THR	678	55.729	12.634	32.107	1.00	46.04
ATOM	5249	OG1	THR	678	54.663	11.676	32.046	1.00	49.79
ATOM	5251	CG2	THR	678	55.160	14.010	32.429	1.00	45.58
ATOM	5252	C	THR	678	56.656	11.221	30.261	1.00	43.81
ATOM	5253	O	THR	678	56.231	10.888	29.158	1.00	45.12

ATOM	5254	N	HIS	679	57.250	10.359	31.076	1.00	41.50
ATOM	5256	CA	HIS	679	57.414	8.971	30.687	1.00	38.39
ATOM	5257	CB	HIS	679	58.390	8.253	31.603	1.00	38.62
ATOM	5258	CG	HIS	679	59.798	8.770	31.524	1.00	41.51
ATOM	5259	CD2	HIS	679	60.456	9.690	32.273	1.00	40.12
ATOM	5260	ND1	HIS	679	60.715	8.296	30.613	1.00	41.18
ATOM	5262	CE1	HIS	679	61.880	8.892	30.806	1.00	39.44
ATOM	5263	NE2	HIS	679	61.747	9.742	31.807	1.00	41.37
ATOM	5265	C	HIS	679	56.068	8.279	30.720	1.00	39.57
ATOM	5266	O	HIS	679	55.909	7.215	30.137	1.00	41.93
ATOM	5267	N	GLN	680	55.108	8.863	31.429	1.00	39.84
ATOM	5269	CA	GLN	680	53.773	8.290	31.483	1.00	38.92
ATOM	5270	CB	GLN	680	53.021	8.705	32.751	1.00	38.21
ATOM	5271	CG	GLN	680	53.518	8.005	34.022	1.00	42.17
ATOM	5272	CD	GLN	680	53.651	6.477	33.878	1.00	43.35
ATOM	5273	OE1	GLN	680	52.686	5.737	34.056	1.00	44.05
ATOM	5274	NE2	GLN	680	54.860	6.010	33.564	1.00	37.17
ATOM	5277	C	GLN	680	53.012	8.674	30.221	1.00	39.33
ATOM	5278	O	GLN	680	52.220	7.883	29.709	1.00	40.26
ATOM	5279	N	SER	681	53.299	9.854	29.673	1.00	38.00
ATOM	5281	CA	SER	681	52.636	10.251	28.441	1.00	37.44
ATOM	5282	CB	SER	681	52.963	11.698	28.078	1.00	37.67
ATOM	5283	OG	SER	681	54.349	11.937	28.102	1.00	38.03
ATOM	5285	C	SER	681	53.095	9.278	27.356	1.00	38.28
ATOM	5286	O	SER	681	52.302	8.866	26.510	1.00	39.41
ATOM	5287	N	ASP	682	54.362	8.866	27.431	1.00	36.81
ATOM	5289	CA	ASP	682	54.920	7.888	26.495	1.00	36.41
ATOM	5290	CB	ASP	682	56.404	7.655	26.765	1.00	37.18
ATOM	5291	CG	ASP	682	57.309	8.584	25.968	1.00	40.08
ATOM	5292	OD1	ASP	682	58.528	8.317	25.959	1.00	41.94
ATOM	5293	OD2	ASP	682	56.824	9.565	25.352	1.00	39.55
ATOM	5294	C	ASP	682	54.180	6.561	26.645	1.00	36.93
ATOM	5295	O	ASP	682	54.005	5.818	25.675	1.00	38.23
ATOM	5296	N	VAL	683	53.742	6.268	27.866	1.00	36.33
ATOM	5298	CA	VAL	683	53.000	5.040	28.143	1.00	36.29
ATOM	5299	CB	VAL	683	52.834	4.820	29.683	1.00	35.29
ATOM	5300	CG1	VAL	683	51.900	3.653	29.989	1.00	34.98
ATOM	5301	CG2	VAL	683	54.198	4.546	30.312	1.00	30.55
ATOM	5302	C	VAL	683	51.648	5.067	27.392	1.00	35.21
ATOM	5303	O	VAL	683	51.223	4.050	26.845	1.00	32.81
ATOM	5304	N	TRP	684	51.027	6.245	27.309	1.00	34.49
ATOM	5306	CA	TRP	684	49.759	6.412	26.602	1.00	36.39
ATOM	5307	CB	TRP	684	49.200	7.825	26.811	1.00	39.30
ATOM	5308	CG	TRP	684	48.006	8.174	25.947	1.00	41.47
ATOM	5309	CD2	TRP	684	46.651	8.381	26.384	1.00	42.41
ATOM	5310	CE2	TRP	684	45.896	8.744	25.247	1.00	41.76
ATOM	5311	CE3	TRP	684	46.004	8.298	27.627	1.00	42.06
ATOM	5312	CD1	TRP	684	48.010	8.410	24.597	1.00	40.55
ATOM	5313	NE1	TRP	684	46.749	8.756	24.175	1.00	42.32
ATOM	5315	CZ2	TRP	684	44.522	9.022	25.315	1.00	41.35
ATOM	5316	CZ3	TRP	684	44.638	8.576	27.692	1.00	41.99
ATOM	5317	CH2	TRP	684	43.917	8.933	26.541	1.00	41.07

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ATOM	5318	C	TRP	684	49.964	6.125	25.115	1.00	36.12
ATOM	5319	O	TRP	684	49.152	5.410	24.511	1.00	38.69
ATOM	5320	N	SER	685	51.029	6.690	24.534	1.00	33.48
ATOM	5322	CA	SER	685	51.395	6.491	23.130	1.00	26.49
ATOM	5323	CB	SER	685	52.636	7.300	22.802	1.00	23.40
ATOM	5324	OG	SER	685	52.403	8.688	22.992	1.00	30.31
ATOM	5326	C	SER	685	51.665	5.015	22.859	1.00	26.25
ATOM	5327	O	SER	685	51.377	4.510	21.782	1.00	28.78
ATOM	5328	N	PHE	686	52.214	4.319	23.846	1.00	28.14
ATOM	5330	CA	PHE	686	52.470	2.884	23.727	1.00	28.53
ATOM	5331	CB	PHE	686	53.245	2.399	24.947	1.00	27.34
ATOM	5332	CG	PHE	686	53.567	0.937	24.917	1.00	29.91
ATOM	5333	CD1	PHE	686	54.424	0.419	23.942	1.00	29.23
ATOM	5334	CD2	PHE	686	53.016	0.075	25.861	1.00	28.28
ATOM	5335	CE1	PHE	686	54.725	-0.936	23.908	1.00	27.65
ATOM	5336	CE2	PHE	686	53.307	-1.274	25.840	1.00	27.18
ATOM	5337	CZ	PHE	686	54.166	-1.787	24.861	1.00	30.06
ATOM	5338	C	PHE	686	51.129	2.117	23.618	1.00	31.42
ATOM	5339	O	PHE	686	51.041	1.096	22.930	1.00	29.05
ATOM	5340	N	GLY	687	50.093	2.623	24.298	1.00	31.18
ATOM	5342	CA	GLY	687	48.783	2.000	24.258	1.00	32.16
ATOM	5343	C	GLY	687	48.276	2.026	22.825	1.00	35.09
ATOM	5344	O	GLY	687	47.805	1.011	22.289	1.00	36.38
ATOM	5345	N	VAL	688	48.378	3.188	22.186	1.00	33.72
ATOM	5347	CA	VAL	688	47.949	3.307	20.808	1.00	30.28
ATOM	5348	CB	VAL	688	47.996	4.761	20.322	1.00	28.62
ATOM	5349	CG1	VAL	688	47.433	4.862	18.905	1.00	26.79
ATOM	5350	CG2	VAL	688	47.202	5.645	21.275	1.00	26.40
ATOM	5351	C	VAL	688	48.823	2.406	19.930	1.00	30.01
ATOM	5352	O	VAL	688	48.324	1.782	18.989	1.00	30.37
ATOM	5353	N	LEU	689	50.108	2.282	20.273	1.00	29.76
ATOM	5355	CA	LEU	689	51.022	1.418	19.510	1.00	29.37
ATOM	5356	CB	LEU	689	52.476	1.577	19.982	1.00	25.78
ATOM	5357	CG	LEU	689	53.564	0.944	19.097	1.00	23.00
ATOM	5358	CD1	LEU	689	54.855	1.741	19.153	1.00	24.44
ATOM	5359	CD2	LEU	689	53.823	-0.471	19.479	1.00	21.63
ATOM	5360	C	LEU	689	50.583	-0.043	19.634	1.00	29.98
ATOM	5361	O	LEU	689	50.708	-0.806	18.678	1.00	28.75
ATOM	5362	N	LEU	690	50.048	-0.409	20.803	1.00	32.38
ATOM	5364	CA	LEU	690	49.562	-1.764	21.060	1.00	32.66
ATOM	5365	CB	LEU	690	49.114	-1.929	22.517	1.00	32.33
ATOM	5366	CG	LEU	690	50.107	-2.192	23.658	1.00	32.00
ATOM	5367	CD1	LEU	690	49.330	-2.201	24.962	1.00	35.74
ATOM	5368	CD2	LEU	690	50.834	-3.513	23.475	1.00	30.76
ATOM	5369	C	LEU	690	48.369	-2.018	20.156	1.00	33.29
ATOM	5370	O	LEU	690	48.248	-3.079	19.550	1.00	35.08
ATOM	5371	N	TRP	691	47.490	-1.026	20.065	1.00	34.28
ATOM	5373	CA	TRP	691	46.304	-1.114	19.221	1.00	33.79
ATOM	5374	CB	TRP	691	45.483	0.172	19.364	1.00	32.68
ATOM	5375	CG	TRP	691	44.147	0.144	18.669	1.00	31.23
ATOM	5376	CD2	TRP	691	43.888	0.490	17.312	1.00	28.11
ATOM	5377	CE2	TRP	691	42.506	0.310	17.089	1.00	29.96

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ATOM	5378	CE3	TRP	691	44.686	0.949	16.257	1.00	28.70
ATOM	5379	CD1	TRP	691	42.936	-0.225	19.208	1.00	29.37
ATOM	5380	NE1	TRP	691	41.951	-0.130	18.265	1.00	30.89
ATOM	5382	CZ2	TRP	691	41.909	0.555	15.845	1.00	29.50
ATOM	5383	CZ3	TRP	691	44.093	1.194	15.021	1.00	27.43
ATOM	5384	CH2	TRP	691	42.719	1.002	14.830	1.00	29.27
ATOM	5385	C	TRP	691	46.744	-1.319	17.763	1.00	34.12
ATOM	5386	O	TRP	691	46.139	-2.088	17.029	1.00	33.88
ATOM	5387	N	GLU	692	47.817	-0.636	17.366	1.00	36.37
ATOM	5389	CA	GLU	692	48.355	-0.723	16.010	1.00	35.35
ATOM	5390	CB	GLU	692	49.532	0.233	15.826	1.00	31.75
ATOM	5391	CG	GLU	692	49.138	1.694	15.746	1.00	32.63
ATOM	5392	CD	GLU	692	50.318	2.585	15.403	1.00	35.28
ATOM	5393	OE1	GLU	692	51.150	2.847	16.301	1.00	37.81
ATOM	5394	OE2	GLU	692	50.430	3.017	14.237	1.00	34.85
ATOM	5395	C	GLU	692	48.810	-2.118	15.658	1.00	35.71
ATOM	5396	O	GLU	692	48.589	-2.570	14.544	1.00	37.26
ATOM	5397	N	ILE	693	49.439	-2.798	16.610	1.00	35.05
ATOM	5399	CA	ILE	693	49.944	-4.153	16.396	1.00	35.00
ATOM	5400	CB	ILE	693	50.843	-4.608	17.575	1.00	35.88
ATOM	5401	CG2	ILE	693	51.275	-6.064	17.400	1.00	36.03
ATOM	5402	CG1	ILE	693	52.081	-3.711	17.669	1.00	34.66
ATOM	5403	CD1	ILE	693	52.814	-3.874	18.943	1.00	35.52
ATOM	5404	C	ILE	693	48.810	-5.153	16.232	1.00	34.29
ATOM	5405	O	ILE	693	48.790	-5.943	15.281	1.00	33.66
ATOM	5406	N	PHE	694	47.837	-5.079	17.127	1.00	34.44
ATOM	5408	CA	PHE	694	46.722	-5.999	17.082	1.00	35.63
ATOM	5409	CB	PHE	694	46.156	-6.167	18.490	1.00	35.26
ATOM	5410	CG	PHE	694	47.158	-6.787	19.428	1.00	35.26
ATOM	5411	CD1	PHE	694	47.796	-6.017	20.389	1.00	33.07
ATOM	5412	CD2	PHE	694	47.574	-8.111	19.237	1.00	31.74
ATOM	5413	CE1	PHE	694	48.837	-6.539	21.137	1.00	31.01
ATOM	5414	CE2	PHE	694	48.614	-8.643	19.982	1.00	31.64
ATOM	5415	CZ	PHE	694	49.254	-7.855	20.934	1.00	31.84
ATOM	5416	C	PHE	694	45.688	-5.771	15.986	1.00	36.62
ATOM	5417	O	PHE	694	44.844	-6.632	15.729	1.00	38.73
ATOM	5418	N	THR	695	45.781	-4.626	15.313	1.00	35.76
ATOM	5420	CA	THR	695	44.898	-4.331	14.191	1.00	34.86
ATOM	5421	CB	THR	695	44.245	-2.929	14.298	1.00	32.81
ATOM	5422	OG1	THR	695	45.246	-1.909	14.211	1.00	31.61
ATOM	5424	CG2	THR	695	43.497	-2.795	15.603	1.00	29.90
ATOM	5425	C	THR	695	45.766	-4.426	12.934	1.00	35.95
ATOM	5426	O	THR	695	45.333	-4.064	11.841	1.00	38.88
ATOM	5427	N	LEU	696	46.993	-4.919	13.119	1.00	34.68
ATOM	5429	CA	LEU	696	47.979	-5.100	12.053	1.00	32.84
ATOM	5430	CB	LEU	696	47.622	-6.294	11.161	1.00	32.65
ATOM	5431	CG	LEU	696	47.493	-7.657	11.838	1.00	30.89
ATOM	5432	CD1	LEU	696	47.315	-8.734	10.785	1.00	31.30
ATOM	5433	CD2	LEU	696	48.718	-7.939	12.659	1.00	30.76
ATOM	5434	C	LEU	696	48.280	-3.872	11.197	1.00	32.43
ATOM	5435	O	LEU	696	48.259	-3.931	9.965	1.00	31.48
ATOM	5436	N	GLY	697	48.597	-2.768	11.867	1.00	33.65

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ATOM	5438	CA	GLY	697	48.940	-1.529	11.188	1.00	32.78
ATOM	5439	C	GLY	697	47.742	-0.641	10.960	1.00	33.06
ATOM	5440	O	GLY	697	47.728	0.172	10.048	1.00	34.74
ATOM	5441	N	GLY	698	46.719	-0.798	11.782	1.00	35.53
ATOM	5443	CA	GLY	698	45.531	0.009	11.612	1.00	36.87
ATOM	5444	C	GLY	698	45.771	1.496	11.753	1.00	34.92
ATOM	5445	O	GLY	698	46.779	1.926	12.299	1.00	34.08
ATOM	5446	N	SER	699	44.814	2.271	11.265	1.00	36.45
ATOM	5448	CA	SER	699	44.858	3.725	11.318	1.00	35.36
ATOM	5449	CB	SER	699	44.363	4.290	9.995	1.00	34.58
ATOM	5450	OG	SER	699	44.126	5.684	10.087	1.00	41.43
ATOM	5452	C	SER	699	43.927	4.146	12.451	1.00	36.53
ATOM	5453	O	SER	699	42.734	3.812	12.438	1.00	37.58
ATOM	5454	N	PRO	700	44.471	4.799	13.491	1.00	36.03
ATOM	5455	CD	PRO	700	45.896	5.028	13.776	1.00	34.58
ATOM	5456	CA	PRO	700	43.630	5.228	14.611	1.00	35.47
ATOM	5457	CB	PRO	700	44.655	5.573	15.694	1.00	34.59
ATOM	5458	CG	PRO	700	45.840	5.990	14.919	1.00	34.18
ATOM	5459	C	PRO	700	42.742	6.411	14.247	1.00	34.66
ATOM	5460	O	PRO	700	43.194	7.363	13.616	1.00	34.39
ATOM	5461	N	TYR	701	41.462	6.293	14.588	1.00	34.11
ATOM	5463	CA	TYR	701	40.459	7.324	14.338	1.00	33.11
ATOM	5464	CB	TYR	701	40.713	8.548	15.225	1.00	38.13
ATOM	5465	CG	TYR	701	40.552	8.272	16.706	1.00	43.52
ATOM	5466	CD1	TYR	701	41.538	8.637	17.616	1.00	44.79
ATOM	5467	CE1	TYR	701	41.387	8.391	18.978	1.00	49.99
ATOM	5468	CD2	TYR	701	39.405	7.647	17.197	1.00	47.59
ATOM	5469	CE2	TYR	701	39.245	7.395	18.552	1.00	49.15
ATOM	5470	CZ	TYR	701	40.237	7.770	19.444	1.00	50.84
ATOM	5471	OH	TYR	701	40.091	7.539	20.804	1.00	54.00
ATOM	5473	C	TYR	701	40.389	7.736	12.877	1.00	30.95
ATOM	5474	O	TYR	701	40.597	8.900	12.534	1.00	30.64
ATOM	5475	N	PRO	702	40.096	6.773	11.985	1.00	30.06
ATOM	5476	CD	PRO	702	39.887	5.336	12.192	1.00	25.47
ATOM	5477	CA	PRO	702	40.014	7.112	10.561	1.00	29.36
ATOM	5478	CB	PRO	702	39.836	5.744	9.899	1.00	25.86
ATOM	5479	CG	PRO	702	39.185	4.946	10.929	1.00	24.42
ATOM	5480	C	PRO	702	38.859	8.045	10.256	1.00	31.49
ATOM	5481	O	PRO	702	37.716	7.794	10.654	1.00	33.50
ATOM	5482	N	GLY	703	39.194	9.151	9.592	1.00	30.85
ATOM	5484	CA	GLY	703	38.210	10.149	9.212	1.00	27.67
ATOM	5485	C	GLY	703	37.985	11.230	10.250	1.00	27.39
ATOM	5486	O	GLY	703	37.270	12.194	9.981	1.00	26.56
ATOM	5487	N	VAL	704	38.627	11.100	11.412	1.00	27.05
ATOM	5489	CA	VAL	704	38.466	12.053	12.505	1.00	28.50
ATOM	5490	CB	VAL	704	38.576	11.364	13.876	1.00	28.95
ATOM	5491	CG1	VAL	704	38.509	12.397	14.990	1.00	29.36
ATOM	5492	CG2	VAL	704	37.475	10.338	14.045	1.00	29.64
ATOM	5493	C	VAL	704	39.473	13.194	12.493	1.00	30.95
ATOM	5494	O	VAL	704	40.669	12.977	12.661	1.00	32.90
ATOM	5495	N	PRO	705	39.001	14.428	12.269	1.00	31.09
ATOM	5496	CD	PRO	705	37.682	14.795	11.728	1.00	31.49

ATOM	5497	CA	PRO	705	39.926	15.561	12.255	1.00	29.66
ATOM	5498	CB	PRO	705	39.152	16.618	11.477	1.00	30.16
ATOM	5499	CG	PRO	705	37.720	16.289	11.778	1.00	33.76
ATOM	5500	C	PRO	705	40.334	16.028	13.654	1.00	29.25
ATOM	5501	O	PRO	705	39.693	15.695	14.659	1.00	24.77
ATOM	5502	N	VAL	706	41.396	16.828	13.690	1.00	32.40
ATOM	5504	CA	VAL	706	41.976	17.355	14.929	1.00	36.51
ATOM	5505	CB	VAL	706	43.023	18.450	14.629	1.00	36.79
ATOM	5506	CG1	VAL	706	43.680	18.903	15.914	1.00	37.79
ATOM	5507	CG2	VAL	706	44.058	17.942	13.653	1.00	37.26
ATOM	5508	C	VAL	706	40.977	17.915	15.943	1.00	38.21
ATOM	5509	O	VAL	706	41.052	17.600	17.130	1.00	37.65
ATOM	5510	N	GLU	707	40.060	18.754	15.467	1.00	40.27
ATOM	5512	CA	GLU	707	39.045	19.360	16.324	1.00	40.57
ATOM	5513	CB	GLU	707	38.186	20.324	15.499	1.00	40.56
ATOM	5514	C	GLU	707	38.164	18.288	16.958	1.00	41.60
ATOM	5515	O	GLU	707	37.871	18.323	18.158	1.00	41.79
ATOM	5516	N	GLU	708	37.784	17.311	16.143	1.00	42.54
ATOM	5518	CA	GLU	708	36.947	16.210	16.576	1.00	44.09
ATOM	5519	CB	GLU	708	36.509	15.398	15.367	1.00	47.61
ATOM	5520	CG	GLU	708	35.687	16.219	14.381	1.00	50.42
ATOM	5521	CD	GLU	708	34.511	16.891	15.042	1.00	55.51
ATOM	5522	OE1	GLU	708	33.856	16.249	15.899	1.00	58.91
ATOM	5523	OE2	GLU	708	34.244	18.067	14.714	1.00	60.06
ATOM	5524	C	GLU	708	37.661	15.338	17.598	1.00	44.63
ATOM	5525	O	GLU	708	37.058	14.893	18.585	1.00	45.12
ATOM	5526	N	LEU	709	38.960	15.141	17.390	1.00	43.72
ATOM	5528	CA	LEU	709	39.768	14.346	18.312	1.00	39.85
ATOM	5529	CB	LEU	709	41.212	14.243	17.823	1.00	34.99
ATOM	5530	CG	LEU	709	42.037	13.359	18.756	1.00	31.80
ATOM	5531	CD1	LEU	709	41.619	11.918	18.598	1.00	29.20
ATOM	5532	CD2	LEU	709	43.495	13.533	18.454	1.00	31.19
ATOM	5533	C	LEU	709	39.751	15.001	19.683	1.00	39.26
ATOM	5534	O	LEU	709	39.646	14.317	20.714	1.00	37.71
ATOM	5535	N	PHE	710	39.872	16.327	19.691	1.00	38.62
ATOM	5537	CA	PHE	710	39.862	17.068	20.942	1.00	41.82
ATOM	5538	CB	PHE	710	40.016	18.567	20.688	1.00	42.02
ATOM	5539	CG	PHE	710	41.383	18.958	20.206	1.00	43.81
ATOM	5540	CD1	PHE	710	42.441	18.043	20.242	1.00	47.07
ATOM	5541	CD2	PHE	710	41.621	20.234	19.718	1.00	42.91
ATOM	5542	CE1	PHE	710	43.716	18.401	19.793	1.00	49.22
ATOM	5543	CE2	PHE	710	42.890	20.602	19.267	1.00	46.73
ATOM	5544	CZ	PHE	710	43.942	19.681	19.307	1.00	48.40
ATOM	5545	C	PHE	710	38.568	16.787	21.698	1.00	43.80
ATOM	5546	O	PHE	710	38.593	16.502	22.904	1.00	44.54
ATOM	5547	N	LYS	711	37.452	16.790	20.968	1.00	44.15
ATOM	5549	CA	LYS	711	36.148	16.539	21.569	1.00	42.60
ATOM	5550	CB	LYS	711	35.029	16.855	20.577	1.00	44.35
ATOM	5551	CG	LYS	711	33.661	16.781	21.200	1.00	48.05
ATOM	5552	CD	LYS	711	32.560	17.205	20.263	1.00	49.23
ATOM	5553	CE	LYS	711	31.212	16.804	20.855	1.00	50.61
ATOM	5554	NZ	LYS	711	30.078	17.204	19.987	1.00	56.56

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ATOM	5558	C	LYS	711	36.045	15.105	22.084	1.00	41.50
ATOM	5559	O	LYS	711	35.589	14.875	23.202	1.00	41.06
ATOM	5560	N	LEU	712	36.489	14.144	21.282	1.00	41.61
ATOM	5562	CA	LEU	712	36.463	12.737	21.687	1.00	43.22
ATOM	5563	CB	LEU	712	37.070	11.841	20.600	1.00	41.69
ATOM	5564	CG	LEU	712	36.246	11.404	19.397	1.00	38.07
ATOM	5565	CD1	LEU	712	37.071	10.460	18.527	1.00	34.55
ATOM	5566	CD2	LEU	712	34.990	10.714	19.891	1.00	37.28
ATOM	5567	C	LEU	712	37.253	12.536	22.982	1.00	43.94
ATOM	5568	O	LEU	712	36.804	11.832	23.900	1.00	41.71
ATOM	5569	N	LEU	713	38.444	13.129	23.029	1.00	45.26
ATOM	5571	CA	LEU	713	39.318	13.022	24.191	1.00	46.47
ATOM	5572	CB	LEU	713	40.647	13.728	23.925	1.00	46.32
ATOM	5573	CG	LEU	713	41.524	13.012	22.889	1.00	44.05
ATOM	5574	CD1	LEU	713	42.853	13.737	22.734	1.00	39.96
ATOM	5575	CD2	LEU	713	41.758	11.571	23.328	1.00	41.78
ATOM	5576	C	LEU	713	38.665	13.519	25.477	1.00	47.50
ATOM	5577	O	LEU	713	38.630	12.789	26.472	1.00	48.26
ATOM	5578	N	LYS	714	38.098	14.725	25.440	1.00	47.08
ATOM	5580	CA	LYS	714	37.419	15.302	26.600	1.00	45.59
ATOM	5581	CB	LYS	714	36.974	16.727	26.293	1.00	47.53
ATOM	5582	CG	LYS	714	38.126	17.661	26.064	1.00	51.33
ATOM	5583	CD	LYS	714	37.647	19.044	25.689	1.00	59.12
ATOM	5584	CE	LYS	714	38.836	19.917	25.273	1.00	64.39
ATOM	5585	NZ	LYS	714	39.843	20.072	26.370	1.00	66.31
ATOM	5589	C	LYS	714	36.217	14.476	27.056	1.00	44.19
ATOM	5590	O	LYS	714	35.895	14.447	28.244	1.00	43.04
ATOM	5591	N	GLU	715	35.565	13.805	26.112	1.00	43.89
ATOM	5593	CA	GLU	715	34.401	12.976	26.424	1.00	44.12
ATOM	5594	CB	GLU	715	33.512	12.785	25.190	1.00	47.40
ATOM	5595	CG	GLU	715	32.860	14.053	24.623	1.00	52.31
ATOM	5596	CD	GLU	715	31.953	13.763	23.427	1.00	56.22
ATOM	5597	OE1	GLU	715	32.121	12.699	22.784	1.00	57.16
ATOM	5598	OE2	GLU	715	31.059	14.588	23.138	1.00	57.32
ATOM	5599	C	GLU	715	34.809	11.605	26.956	1.00	42.47
ATOM	5600	O	GLU	715	33.964	10.718	27.094	1.00	41.03
ATOM	5601	N	GLY	716	36.101	11.419	27.201	1.00	41.06
ATOM	5603	CA	GLY	716	36.593	10.150	27.718	1.00	41.58
ATOM	5604	C	GLY	716	36.548	8.985	26.739	1.00	41.60
ATOM	5605	O	GLY	716	36.640	7.816	27.141	1.00	38.34
ATOM	5606	N	HIS	717	36.469	9.303	25.450	1.00	42.80
ATOM	5608	CA	HIS	717	36.398	8.278	24.420	1.00	45.03
ATOM	5609	CB	HIS	717	36.082	8.894	23.052	1.00	46.28
ATOM	5610	CG	HIS	717	35.987	7.887	21.940	1.00	48.73
ATOM	5611	CD2	HIS	717	34.941	7.157	21.483	1.00	48.67
ATOM	5612	ND1	HIS	717	37.071	7.521	21.169	1.00	49.33
ATOM	5614	CE1	HIS	717	36.701	6.607	20.290	1.00	45.65
ATOM	5615	NE2	HIS	717	35.410	6.370	20.460	1.00	45.87
ATOM	5617	C	HIS	717	37.662	7.448	24.324	1.00	46.84
ATOM	5618	O	HIS	717	38.767	7.980	24.319	1.00	48.06
ATOM	5619	N	ARG	718	37.478	6.138	24.217	1.00	48.75
ATOM	5621	CA	ARG	718	38.573	5.181	24.091	1.00	49.16

ATOM	5622	CB	ARG	718	38.694	4.345	25.370	1.00	46.96
ATOM	5623	CG	ARG	718	39.005	5.164	26.617	1.00	49.78
ATOM	5624	CD	ARG	718	40.344	5.891	26.474	1.00	52.81
ATOM	5625	NE	ARG	718	40.724	6.639	27.672	1.00	52.99
ATOM	5627	CZ	ARG	718	40.598	7.961	27.817	1.00	53.38
ATOM	5628	NH1	ARG	718	40.094	8.705	26.836	1.00	52.33
ATOM	5631	NH2	ARG	718	41.025	8.553	28.928	1.00	49.30
ATOM	5634	C	ARG	718	38.257	4.293	22.878	1.00	50.73
ATOM	5635	O	ARG	718	37.086	4.003	22.601	1.00	51.78
ATOM	5636	N	MET	719	39.286	3.899	22.136	1.00	50.83
ATOM	5638	CA	MET	719	39.086	3.072	20.948	1.00	50.56
ATOM	5639	CB	MET	719	40.355	3.013	20.094	1.00	48.85
ATOM	5640	CG	MET	719	40.748	4.325	19.438	1.00	45.25
ATOM	5641	SD	MET	719	42.152	4.119	18.335	1.00	43.24
ATOM	5642	CE	MET	719	43.471	4.066	19.465	1.00	36.42
ATOM	5643	C	MET	719	38.649	1.671	21.312	1.00	51.07
ATOM	5644	O	MET	719	39.087	1.132	22.325	1.00	48.42
ATOM	5645	N	ASP	720	37.797	1.096	20.462	1.00	53.92
ATOM	5647	CA	ASP	720	37.254	-0.253	20.648	1.00	55.90
ATOM	5648	CB	ASP	720	36.221	-0.597	19.553	1.00	57.16
ATOM	5649	CG	ASP	720	34.998	0.320	19.552	1.00	59.05
ATOM	5650	OD1	ASP	720	34.951	1.316	20.312	1.00	63.29
ATOM	5651	OD2	ASP	720	34.074	0.042	18.758	1.00	54.85
ATOM	5652	C	ASP	720	38.326	-1.343	20.638	1.00	55.89
ATOM	5653	O	ASP	720	39.397	-1.190	20.027	1.00	55.28
ATOM	5654	N	LYS	721	38.008	-2.450	21.304	1.00	56.09
ATOM	5656	CA	LYS	721	38.892	-3.605	21.370	1.00	56.46
ATOM	5657	CB	LYS	721	38.344	-4.606	22.378	1.00	58.16
ATOM	5658	CG	LYS	721	39.005	-5.977	22.316	1.00	62.49
ATOM	5659	CD	LYS	721	38.449	-6.873	23.401	1.00	66.40
ATOM	5660	CE	LYS	721	38.474	-8.329	22.995	1.00	68.27
ATOM	5661	NZ	LYS	721	38.107	-9.194	24.156	1.00	75.61
ATOM	5665	C	LYS	721	38.930	-4.241	19.985	1.00	56.00
ATOM	5666	O	LYS	721	37.884	-4.532	19.403	1.00	59.26
ATOM	5667	N	PRO	722	40.133	-4.439	19.423	1.00	54.10
ATOM	5668	CD	PRO	722	41.461	-3.968	19.836	1.00	53.72
ATOM	5669	CA	PRO	722	40.208	-5.046	18.094	1.00	51.82
ATOM	5670	CB	PRO	722	41.702	-4.953	17.759	1.00	49.09
ATOM	5671	CG	PRO	722	42.143	-3.768	18.501	1.00	49.06
ATOM	5672	C	PRO	722	39.765	-6.498	18.123	1.00	50.10
ATOM	5673	O	PRO	722	39.678	-7.120	19.188	1.00	48.82
ATOM	5674	N	SER	723	39.453	-7.020	16.945	1.00	49.87
ATOM	5676	CA	SER	723	39.079	-8.410	16.814	1.00	50.27
ATOM	5677	CB	SER	723	38.396	-8.643	15.473	1.00	48.56
ATOM	5678	OG	SER	723	39.273	-8.323	14.404	1.00	48.93
ATOM	5680	C	SER	723	40.414	-9.144	16.872	1.00	51.33
ATOM	5681	O	SER	723	41.400	-8.679	16.311	1.00	51.18
ATOM	5682	N	ASN	724	40.445	-10.284	17.551	1.00	54.65
ATOM	5684	CA	ASN	724	41.673	-11.062	17.706	1.00	56.76
ATOM	5685	CB	ASN	724	42.370	-11.286	16.359	1.00	58.96
ATOM	5686	CG	ASN	724	41.698	-12.345	15.543	1.00	62.08
ATOM	5687	OD1	ASN	724	41.645	-13.508	15.948	1.00	67.56

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ATOM	5688	ND2	ASN	724	41.154	-11.960	14.403	1.00	60.12
ATOM	5691	C	ASN	724	42.622	-10.381	18.683	1.00	57.26
ATOM	5692	O	ASN	724	43.786	-10.131	18.383	1.00	58.40
ATOM	5693	N	CYS	725	42.089	-10.045	19.845	1.00	57.58
ATOM	5695	CA	CYS	725	42.852	-9.418	20.908	1.00	57.02
ATOM	5696	CB	CYS	725	42.835	-7.885	20.803	1.00	55.65
ATOM	5697	SG	CYS	725	43.782	-7.034	22.119	1.00	52.17
ATOM	5698	C	CYS	725	42.158	-9.884	22.177	1.00	56.53
ATOM	5699	O	CYS	725	40.927	-9.954	22.240	1.00	55.99
ATOM	5700	N	THR	726	42.957	-10.279	23.155	1.00	56.09
ATOM	5702	CA	THR	726	42.453	-10.773	24.423	1.00	57.09
ATOM	5703	CB	THR	726	43.551	-11.579	25.129	1.00	57.12
ATOM	5704	OG1	THR	726	44.588	-10.696	25.562	1.00	59.14
ATOM	5706	CG2	THR	726	44.152	-12.587	24.154	1.00	55.09
ATOM	5707	C	THR	726	41.994	-9.608	25.288	1.00	57.58
ATOM	5708	O	THR	726	42.555	-8.518	25.195	1.00	58.49
ATOM	5709	N	ASN	727	40.979	-9.832	26.120	1.00	58.48
ATOM	5711	CA	ASN	727	40.482	-8.774	26.986	1.00	58.74
ATOM	5712	CB	ASN	727	39.331	-9.267	27.864	1.00	66.81
ATOM	5713	CG	ASN	727	39.674	-10.534	28.631	1.00	76.72
ATOM	5714	OD1	ASN	727	40.778	-10.689	29.161	1.00	80.48
ATOM	5715	ND2	ASN	727	38.716	-11.458	28.689	1.00	82.39
ATOM	5718	C	ASN	727	41.606	-8.238	27.852	1.00	55.48
ATOM	5719	O	ASN	727	41.589	-7.080	28.255	1.00	51.24
ATOM	5720	N	GLU	728	42.589	-9.099	28.114	1.00	55.37
ATOM	5722	CA	GLU	728	43.757	-8.739	28.913	1.00	55.53
ATOM	5723	CB	GLU	728	44.611	-9.983	29.198	1.00	55.75
ATOM	5724	CG	GLU	728	45.881	-9.699	30.006	1.00	58.24
ATOM	5725	CD	GLU	728	46.606	-10.958	30.463	1.00	58.16
ATOM	5726	OE1	GLU	728	46.977	-11.796	29.611	1.00	56.39
ATOM	5727	OE2	GLU	728	46.816	-11.102	31.686	1.00	58.35
ATOM	5728	C	GLU	728	44.564	-7.685	28.153	1.00	54.11
ATOM	5729	O	GLU	728	44.790	-6.575	28.654	1.00	55.67
ATOM	5730	N	LEU	729	44.954	-8.020	26.926	1.00	49.65
ATOM	5732	CA	LEU	729	45.715	-7.106	26.086	1.00	46.10
ATOM	5733	CB	LEU	729	46.038	-7.766	24.742	1.00	39.77
ATOM	5734	CG	LEU	729	47.136	-8.836	24.848	1.00	36.12
ATOM	5735	CD1	LEU	729	47.118	-9.757	23.673	1.00	34.89
ATOM	5736	CD2	LEU	729	48.498	-8.193	24.987	1.00	33.47
ATOM	5737	C	LEU	729	44.950	-5.794	25.908	1.00	45.05
ATOM	5738	O	LEU	729	45.522	-4.713	26.019	1.00	45.58
ATOM	5739	N	TYR	730	43.640	-5.884	25.722	1.00	43.53
ATOM	5741	CA	TYR	730	42.831	-4.692	25.557	1.00	43.57
ATOM	5742	CB	TYR	730	41.414	-5.064	25.097	1.00	41.49
ATOM	5743	CG	TYR	730	40.492	-3.870	24.951	1.00	40.28
ATOM	5744	CD1	TYR	730	40.763	-2.865	24.013	1.00	36.86
ATOM	5745	CE1	TYR	730	39.937	-1.752	23.891	1.00	36.21
ATOM	5746	CD2	TYR	730	39.361	-3.730	25.768	1.00	39.44
ATOM	5747	CE2	TYR	730	38.522	-2.616	25.654	1.00	38.13
ATOM	5748	CZ	TYR	730	38.817	-1.632	24.712	1.00	38.79
ATOM	5749	OH	TYR	730	37.974	-0.542	24.575	1.00	40.32
ATOM	5751	C	TYR	730	42.806	-3.866	26.856	1.00	44.45

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ATOM	5752	O	TYR	730	42.786	-2.632	26.818	1.00	43.45
ATOM	5753	N	MET	731	42.798	-4.534	28.006	1.00	46.44
ATOM	5755	CA	MET	731	42.805	-3.812	29.279	1.00	48.59
ATOM	5756	CB	MET	731	42.516	-4.748	30.447	1.00	54.69
ATOM	5757	CG	MET	731	41.132	-5.387	30.398	1.00	62.68
ATOM	5758	SD	MET	731	39.781	-4.189	30.392	1.00	70.49
ATOM	5759	CE	MET	731	39.492	-4.012	32.209	1.00	72.27
ATOM	5760	C	MET	731	44.167	-3.139	29.450	1.00	46.48
ATOM	5761	O	MET	731	44.280	-2.085	30.086	1.00	44.91
ATOM	5762	N	MET	732	45.202	-3.751	28.881	1.00	43.80
ATOM	5764	CA	MET	732	46.538	-3.167	28.939	1.00	43.03
ATOM	5765	CB	MET	732	47.593	-4.104	28.322	1.00	39.44
ATOM	5766	CG	MET	732	49.028	-3.578	28.427	1.00	36.02
ATOM	5767	SD	MET	732	50.312	-4.775	27.979	1.00	36.47
ATOM	5768	CE	MET	732	50.547	-5.573	29.530	1.00	41.29
ATOM	5769	C	MET	732	46.474	-1.833	28.188	1.00	42.08
ATOM	5770	O	MET	732	46.995	-0.827	28.659	1.00	42.14
ATOM	5771	N	MET	733	45.775	-1.822	27.054	1.00	43.14
ATOM	5773	CA	MET	733	45.608	-0.609	26.257	1.00	42.24
ATOM	5774	CB	MET	733	44.852	-0.877	24.947	1.00	41.41
ATOM	5775	CG	MET	733	45.607	-1.730	23.938	1.00	40.23
ATOM	5776	SD	MET	733	44.669	-2.025	22.419	1.00	38.02
ATOM	5777	CE	MET	733	45.183	-3.724	21.982	1.00	28.12
ATOM	5778	C	MET	733	44.820	0.392	27.074	1.00	41.68
ATOM	5779	O	MET	733	45.215	1.550	27.196	1.00	43.78
ATOM	5780	N	ARG	734	43.713	-0.053	27.655	1.00	42.59
ATOM	5782	CA	ARG	734	42.893	0.839	28.467	1.00	42.92
ATOM	5783	CB	ARG	734	41.642	-0.119	28.966	1.00	42.35
ATOM	5784	CG	ARG	734	40.753	-0.374	27.852	1.00	39.76
ATOM	5785	CD	ARG	734	40.360	0.763	26.959	1.00	41.83
ATOM	5786	NE	ARG	734	39.535	1.745	27.653	1.00	45.36
ATOM	5788	CZ	ARG	734	38.207	1.693	27.708	1.00	50.22
ATOM	5789	NH1	ARG	734	37.542	0.708	27.117	1.00	51.18
ATOM	5792	NH2	ARG	734	37.534	2.642	28.346	1.00	53.24
ATOM	5795	C	ARG	734	43.719	1.385	29.630	1.00	42.42
ATOM	5796	C	ARG	734	43.610	2.571	29.969	1.00	42.59
ATOM	5797	N	ASP	735	44.591	0.544	30.187	1.00	41.40
ATOM	5799	CA	ASP	735	45.464	0.959	31.286	1.00	43.33
ATOM	5800	CB	ASP	735	46.337	-0.194	31.755	1.00	48.28
ATOM	5801	CG	ASP	735	45.556	-1.256	32.496	1.00	54.86
ATOM	5802	OD1	ASP	735	45.903	-2.451	32.322	1.00	53.49
ATOM	5803	OD2	ASP	735	44.612	-0.900	33.245	1.00	55.59
ATOM	5804	C	ASP	735	46.365	2.107	30.840	1.00	42.65
ATOM	5805	O	ASP	735	46.484	3.124	31.543	1.00	44.03
ATOM	5806	N	CYS	736	47.021	1.926	29.693	1.00	38.83
ATOM	5808	CA	CYS	736	47.896	2.952	29.140	1.00	35.90
ATOM	5809	CB	CYS	736	48.545	2.468	27.858	1.00	33.62
ATOM	5810	SG	CYS	736	49.634	1.087	28.104	1.00	33.92
ATOM	5811	C	CYS	736	47.100	4.208	28.855	1.00	35.96
ATOM	5812	O	CYS	736	47.651	5.309	28.830	1.00	35.59
ATOM	5813	N	TRP	737	45.793	4.039	28.668	1.00	38.02
ATOM	5815	CA	TRP	737	44.906	5.156	28.372	1.00	40.14

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ATOM	5816	CB	TRP	737	43.910	4.766	27.274	1.00	40.93
ATOM	5817	CG	TRP	737	44.563	4.379	25.977	1.00	42.36
ATOM	5818	CD2	TRP	737	44.018	3.518	24.969	1.00	43.84
ATOM	5819	CE2	TRP	737	44.972	3.437	23.929	1.00	46.42
ATOM	5820	CE3	TRP	737	42.817	2.806	24.845	1.00	42.43
ATOM	5821	CD1	TRP	737	45.793	4.775	25.519	1.00	42.57
ATOM	5822	NE1	TRP	737	46.043	4.214	24.292	1.00	44.22
ATOM	5824	CZ2	TRP	737	44.756	2.666	22.773	1.00	44.97
ATOM	5825	CZ3	TRP	737	42.606	2.042	23.699	1.00	40.74
ATOM	5826	CH2	TRP	737	43.571	1.978	22.682	1.00	40.75
ATOM	5827	C	TRP	737	44.157	5.706	29.584	1.00	40.62
ATOM	5828	O	TRP	737	43.085	6.285	29.437	1.00	41.37
ATOM	5829	N	HIS	738	44.706	5.533	30.783	1.00	42.09
ATOM	5831	CA	HIS	738	44.044	6.059	31.966	1.00	43.78
ATOM	5832	CB	HIS	738	44.635	5.463	33.248	1.00	46.52
ATOM	5833	CG	HIS	738	43.878	5.844	34.486	1.00	52.24
ATOM	5834	CD2	HIS	738	43.599	7.053	35.025	1.00	50.95
ATOM	5835	ND1	HIS	738	43.271	4.914	35.299	1.00	56.16
ATOM	5837	CE1	HIS	738	42.643	5.536	36.285	1.00	57.23
ATOM	5838	NE2	HIS	738	42.827	6.835	36.141	1.00	53.22
ATOM	5840	C	HIS	738	44.183	7.577	31.964	1.00	42.81
ATOM	5841	O	HIS	738	45.235	8.093	31.654	1.00	42.12
ATOM	5842	N	ALA	739	43.121	8.285	32.324	1.00	45.66
ATOM	5844	CA	ALA	739	43.130	9.750	32.350	1.00	49.42
ATOM	5845	CB	ALA	739	41.739	10.262	32.681	1.00	53.04
ATOM	5846	C	ALA	739	44.167	10.380	33.291	1.00	50.18
ATOM	5847	O	ALA	739	44.710	11.450	33.006	1.00	51.86
ATOM	5848	N	VAL	740	44.322	9.780	34.466	1.00	49.96
ATOM	5850	CA	VAL	740	45.299	10.219	35.467	1.00	50.17
ATOM	5851	CB	VAL	740	44.828	9.849	36.881	1.00	50.33
ATOM	5852	CG1	VAL	740	45.880	10.209	37.896	1.00	51.40
ATOM	5853	CG2	VAL	740	43.534	10.559	37.193	1.00	50.86
ATOM	5854	C	VAL	740	46.626	9.497	35.196	1.00	49.81
ATOM	5855	O	VAL	740	46.749	8.295	35.472	1.00	49.85
ATOM	5856	N	PRO	741	47.646	10.230	34.713	1.00	47.92
ATOM	5857	CD	PRO	741	47.618	11.683	34.476	1.00	46.97
ATOM	5858	CA	PRO	741	48.968	9.686	34.393	1.00	46.47
ATOM	5859	CB	PRO	741	49.796	10.941	34.134	1.00	44.38
ATOM	5860	CG	PRO	741	48.800	11.877	33.561	1.00	44.86
ATOM	5861	C	PRO	741	49.593	8.815	35.480	1.00	47.21
ATOM	5862	O	PRO	741	50.243	7.816	35.176	1.00	46.77
ATOM	5863	N	SER	742	49.380	9.181	36.741	1.00	48.87
ATOM	5865	CA	SER	742	49.939	8.430	37.860	1.00	50.19
ATOM	5866	CB	SER	742	49.753	9.203	39.166	1.00	51.87
ATOM	5867	OG	SER	742	48.389	9.514	39.391	1.00	54.19
ATOM	5869	C	SER	742	49.331	7.040	38.010	1.00	51.30
ATOM	5870	O	SER	742	49.863	6.192	38.723	1.00	51.14
ATOM	5871	N	GLN	743	48.207	6.814	37.343	1.00	53.07
ATOM	5873	CA	GLN	743	47.531	5.531	37.414	1.00	53.50
ATOM	5874	CB	GLN	743	46.015	5.745	37.548	1.00	59.34
ATOM	5875	CG	GLN	743	45.412	5.307	38.898	1.00	66.19
ATOM	5876	CD	GLN	743	46.133	5.896	40.106	1.00	70.07

ATOM	5877	OE1	GLN	743	46.750	5.170	40.885	1.00	73.86
ATOM	5878	NE2	GLN	743	46.047	7.209	40.273	1.00	72.01
ATOM	5881	C	GLN	743	47.850	4.613	36.236	1.00	51.14
ATOM	5882	O	GLN	743	47.504	3.425	36.266	1.00	51.79
ATOM	5883	N	ARG	744	48.484	5.153	35.196	1.00	48.31
ATOM	5885	CA	ARG	744	48.849	4.343	34.027	1.00	45.49
ATOM	5886	CB	ARG	744	49.326	5.224	32.869	1.00	40.33
ATOM	5887	CG	ARG	744	48.322	6.200	32.324	1.00	36.32
ATOM	5888	CD	ARG	744	48.944	7.100	31.262	1.00	28.55
ATOM	5889	NE	ARG	744	48.050	8.203	30.961	1.00	28.86
ATOM	5891	CZ	ARG	744	48.429	9.409	30.547	1.00	30.58
ATOM	5892	NH1	ARG	744	49.707	9.700	30.357	1.00	26.02
ATOM	5895	NH2	ARG	744	47.516	10.354	30.386	1.00	30.62
ATOM	5898	C	ARG	744	50.016	3.454	34.452	1.00	47.35
ATOM	5899	O	ARG	744	50.794	3.824	35.334	1.00	52.01
ATOM	5900	N	PRO	745	50.133	2.251	33.869	1.00	46.36
ATOM	5901	CD	PRO	745	49.248	1.559	32.921	1.00	45.54
ATOM	5902	CA	PRO	745	51.261	1.402	34.271	1.00	43.41
ATOM	5903	CB	PRO	745	50.972	0.078	33.547	1.00	41.77
ATOM	5904	CG	PRO	745	50.155	0.491	32.354	1.00	42.26
ATOM	5905	C	PRO	745	52.590	2.007	33.822	1.00	40.30
ATOM	5906	O	PRO	745	52.621	2.905	32.990	1.00	39.73
ATOM	5907	N	THR	746	53.679	1.570	34.433	1.00	39.14
ATOM	5909	CA	THR	746	54.997	2.056	34.039	1.00	38.35
ATOM	5910	CB	THR	746	55.992	2.104	35.249	1.00	36.75
ATOM	5911	OG1	THR	746	56.202	0.776	35.769	1.00	32.25
ATOM	5913	CG2	THR	746	55.477	3.037	36.341	1.00	30.31
ATOM	5914	C	THR	746	55.568	1.102	32.987	1.00	37.90
ATOM	5915	O	THR	746	55.185	-0.068	32.938	1.00	37.99
ATOM	5916	N	PHE	747	56.490	1.584	32.157	1.00	35.94
ATOM	5918	CA	PHE	747	57.106	0.716	31.161	1.00	35.00
ATOM	5919	CB	PHE	747	58.124	1.469	30.309	1.00	30.45
ATOM	5920	CG	PHE	747	57.512	2.174	29.142	1.00	27.61
ATOM	5921	CD1	PHE	747	56.950	1.450	28.103	1.00	23.68
ATOM	5922	CD2	PHE	747	57.468	3.556	29.094	1.00	27.97
ATOM	5923	CE1	PHE	747	56.352	2.088	27.033	1.00	23.56
ATOM	5924	CE2	PHE	747	56.869	4.209	28.027	1.00	26.92
ATOM	5925	CZ	PHE	747	56.312	3.470	26.995	1.00	26.21
ATOM	5926	C	PHE	747	57.766	-0.477	31.826	1.00	36.37
ATOM	5927	O	PHE	747	57.920	-1.525	31.219	1.00	37.11
ATOM	5928	N	LYS	748	58.177	-0.312	33.075	1.00	39.68
ATOM	5930	CA	LYS	748	58.797	-1.411	33.807	1.00	42.20
ATOM	5931	CB	LYS	748	59.433	-0.895	35.095	1.00	46.17
ATOM	5932	CG	LYS	748	59.978	-1.991	35.984	1.00	54.78
ATOM	5933	CD	LYS	748	60.794	-1.428	37.135	1.00	58.53
ATOM	5934	CE	LYS	748	61.239	-2.537	38.075	1.00	59.33
ATOM	5935	NZ	LYS	748	62.167	-2.025	39.120	1.00	62.36
ATOM	5939	C	LYS	748	57.723	-2.463	34.111	1.00	42.78
ATOM	5940	O	LYS	748	57.998	-3.664	34.075	1.00	37.97
ATOM	5941	N	GLN	749	56.503	-1.992	34.392	1.00	43.27
ATOM	5943	CA	GLN	749	55.365	-2.866	34.671	1.00	43.39
ATOM	5944	CB	GLN	749	54.146	-2.056	35.146	1.00	47.37

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ATOM	5945	CG	GLN	749	54.236	-1.504	36.569	1.00	51.86
ATOM	5946	CD	GLN	749	53.036	-0.639	36.938	1.00	54.76
ATOM	5947	OE1	GLN	749	53.181	0.504	37.350	1.00	58.36
ATOM	5948	NE2	GLN	749	51.846	-1.179	36.769	1.00	59.25
ATOM	5951	C	GLN	749	55.006	-3.607	33.389	1.00	41.66
ATOM	5952	O	GLN	749	54.978	-4.841	33.355	1.00	40.25
ATOM	5953	N	LEU	750	54.759	-2.843	32.327	1.00	41.47
ATOM	5955	CA	LEU	750	54.398	-3.387	31.018	1.00	40.00
ATOM	5956	CB	LEU	750	54.366	-2.279	29.966	1.00	40.55
ATOM	5957	CG	LEU	750	53.316	-1.174	30.112	1.00	39.94
ATOM	5958	CD1	LEU	750	53.714	0.019	29.257	1.00	41.03
ATOM	5959	CD2	LEU	750	51.952	-1.696	29.722	1.00	37.80
ATOM	5960	C	LEU	750	55.383	-4.452	30.581	1.00	39.61
ATOM	5961	O	LEU	750	54.990	-5.470	30.027	1.00	42.08
ATOM	5962	N	VAL	751	56.670	-4.207	30.804	1.00	40.63
ATOM	5964	CA	VAL	751	57.691	-5.177	30.422	1.00	39.65
ATOM	5965	CB	VAL	751	59.115	-4.639	30.677	1.00	33.44
ATOM	5966	CG1	VAL	751	60.142	-5.694	30.351	1.00	31.57
ATOM	5967	CG2	VAL	751	59.372	-3.433	29.825	1.00	25.19
ATOM	5968	C	VAL	751	57.458	-6.468	31.204	1.00	43.58
ATOM	5969	O	VAL	751	57.530	-7.563	30.646	1.00	44.81
ATOM	5970	N	GLU	752	57.116	-6.339	32.481	1.00	46.24
ATOM	5972	CA	GLU	752	56.869	-7.518	33.301	1.00	50.55
ATOM	5973	CB	GLU	752	56.781	-7.137	34.783	1.00	53.70
ATOM	5974	CG	GLU	752	58.090	-6.541	35.310	1.00	56.60
ATOM	5975	CD	GLU	752	58.079	-6.243	36.792	1.00	56.20
ATOM	5976	OE1	GLU	752	58.387	-5.092	37.178	1.00	53.45
ATOM	5977	OE2	GLU	752	57.789	-7.170	37.573	1.00	60.28
ATOM	5978	C	GLU	752	55.622	-8.275	32.837	1.00	50.90
ATOM	5979	O	GLU	752	55.689	-9.474	32.555	1.00	51.03
ATOM	5980	N	ASP	753	54.501	-7.570	32.708	1.00	51.12
ATOM	5982	CA	ASP	753	53.251	-8.184	32.265	1.00	48.76
ATOM	5983	CB	ASP	753	52.122	-7.160	32.249	1.00	51.11
ATOM	5984	CG	ASP	753	51.646	-6.805	33.636	1.00	54.97
ATOM	5985	OD1	ASP	753	51.592	-7.715	34.495	1.00	58.37
ATOM	5986	OD2	ASP	753	51.319	-5.618	33.864	1.00	56.38
ATOM	5987	C	ASP	753	53.381	-8.790	30.881	1.00	48.02
ATOM	5988	O	ASP	753	52.991	-9.935	30.672	1.00	48.32
ATOM	5989	N	LEU	754	53.925	-8.020	29.940	1.00	45.16
ATOM	5991	CA	LEU	754	54.111	-8.490	28.571	1.00	44.82
ATOM	5992	CB	LEU	754	54.696	-7.387	27.691	1.00	42.70
ATOM	5993	CG	LEU	754	53.736	-6.263	27.298	1.00	42.92
ATOM	5994	CD1	LEU	754	54.500	-5.236	26.495	1.00	41.44
ATOM	5995	CD2	LEU	754	52.537	-6.822	26.502	1.00	42.86
ATOM	5996	C	LEU	754	55.001	-9.716	28.529	1.00	46.00
ATOM	5997	O	LEU	754	54.815	-10.606	27.708	1.00	45.88
ATOM	5998	N	ASP	755	55.975	-9.752	29.424	1.00	47.37
ATOM	6000	CA	ASP	755	56.889	-10.873	29.516	1.00	48.88
ATOM	6001	CB	ASP	755	57.898	-10.584	30.628	1.00	49.89
ATOM	6002	CG	ASP	755	58.998	-11.616	30.717	1.00	51.73
ATOM	6003	OD1	ASP	755	59.640	-11.680	31.785	1.00	55.47
ATOM	6004	OD2	ASP	755	59.236	-12.354	29.738	1.00	50.98

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ATOM	6005	C	ASP	755	56.024	-12.093	29.864	1.00	51.26
ATOM	6006	O	ASP	755	56.021	-13.107	29.155	1.00	50.49
ATOM	6007	N	ARG	756	55.227	-11.940	30.917	1.00	52.15
ATOM	6009	CA	ARG	756	54.332	-12.989	31.385	1.00	53.30
ATOM	6010	CB	ARG	756	53.556	-12.501	32.611	1.00	54.54
ATOM	6011	CG	ARG	756	52.389	-13.380	33.029	1.00	54.26
ATOM	6012	CD	ARG	756	51.672	-12.772	34.215	1.00	56.76
ATOM	6013	NE	ARG	756	51.293	-11.382	33.969	1.00	61.39
ATOM	6015	CZ	ARG	756	50.259	-11.002	33.221	1.00	62.60
ATOM	6016	NH1	ARG	756	49.487	-11.909	32.642	1.00	61.18
ATOM	6019	NH2	ARG	756	49.986	-9.711	33.064	1.00	63.72
ATOM	6022	C	ARG	756	53.357	-13.420	30.297	1.00	53.03
ATOM	6023	O	ARG	756	53.243	-14.607	30.000	1.00	54.82
ATOM	6024	N	ILE	757	52.687	-12.452	29.680	1.00	51.18
ATOM	6026	CA	ILE	757	51.709	-12.732	28.630	1.00	48.68
ATOM	6027	CB	ILE	757	51.025	-11.435	28.120	1.00	47.88
ATOM	6028	CG2	ILE	757	50.112	-11.752	26.953	1.00	45.56
ATOM	6029	CG1	ILE	757	50.247	-10.763	29.258	1.00	47.77
ATOM	6030	CD1	ILE	757	49.651	-9.414	28.914	1.00	46.00
ATOM	6031	C	ILE	757	52.314	-13.482	27.449	1.00	48.30
ATOM	6032	O	ILE	757	51.694	-14.409	26.937	1.00	45.61
ATOM	6033	N	VAL	758	53.523	-13.094	27.038	1.00	48.88
ATOM	6035	CA	VAL	758	54.202	-13.734	25.912	1.00	49.96
ATOM	6036	CB	VAL	758	55.602	-13.101	25.615	1.00	47.80
ATOM	6037	CG1	VAL	758	56.313	-13.864	24.502	1.00	44.17
ATOM	6038	CG2	VAL	758	55.461	-11.660	25.188	1.00	46.65
ATOM	6039	C	VAL	758	54.378	-15.217	26.196	1.00	54.00
ATOM	6040	O	VAL	758	54.218	-16.050	25.306	1.00	53.52
ATOM	6041	N	ALA	759	54.697	-15.540	27.445	1.00	57.83
ATOM	6043	CA	ALA	759	54.898	-16.926	27.844	1.00	61.94
ATOM	6044	CB	ALA	759	55.447	-16.987	29.257	1.00	62.30
ATOM	6045	C	ALA	759	53.592	-17.702	27.761	1.00	65.09
ATOM	6046	O	ALA	759	53.555	-18.823	27.254	1.00	66.39
ATOM	6047	N	LEU	760	52.519	-17.090	28.248	1.00	66.99
ATOM	6049	CA	LEU	760	51.209	-17.720	28.246	1.00	68.78
ATOM	6050	CB	LEU	760	50.314	-17.090	29.320	1.00	68.07
ATOM	6051	CG	LEU	760	50.729	-17.330	30.777	1.00	67.01
ATOM	6052	CD1	LEU	760	49.808	-16.563	31.722	1.00	67.93
ATOM	6053	CD2	LEU	760	50.701	-18.819	31.083	1.00	65.17
ATOM	6054	C	LEU	760	50.510	-17.666	26.892	1.00	71.19
ATOM	6055	O	LEU	760	49.342	-18.039	26.787	1.00	73.15
ATOM	6056	N	THR	761	51.210	-17.201	25.860	1.00	73.38
ATOM	6058	CA	THR	761	50.626	-17.113	24.518	1.00	73.92
ATOM	6059	CB	THR	761	50.963	-15.760	23.829	1.00	72.65
ATOM	6060	OG1	THR	761	50.353	-14.690	24.555	1.00	74.44
ATOM	6062	CG2	THR	761	50.435	-15.731	22.420	1.00	70.32
ATOM	6063	C	THR	761	51.080	-18.276	23.636	1.00	74.66
ATOM	6064	O	THR	761	52.276	-18.520	23.463	1.00	75.08
ATOM	6065	SG	CYS	1603	19.100	-9.073	19.903	0.50	30.84 PRT2
ATOM	6066	CG	MET	534	69.385	12.295	23.393	0.50	33.69 PRT2
ATOM	6067	SD	MET	534	69.112	13.312	24.832	0.50	34.44 PRT2
ATOM	6068	CE	MET	534	70.067	12.429	26.060	0.50	36.92 PRT2

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ATOM	6069	SG	CYS	603	56.370	-7.959	16.451	0.50	41.20	PRT2
ATOM	2716	OH2	TIP3	1	71.864	25.128	2.721	1.00	26.20	
ATOM	2719	OH2	TIP3	2	39.862	4.160	16.115	1.00	42.43	
ATOM	2722	OH2	TIP3	3	83.875	19.969	10.572	1.00	23.41	
ATOM	2725	OH2	TIP3	4	83.585	20.356	7.953	1.00	30.15	
ATOM	2728	OH2	TIP3	5	75.100	16.407	6.948	1.00	46.78	
ATOM	2731	OH2	TIP3	6	86.616	19.701	9.707	1.00	44.37	
ATOM	2734	OH2	TIP3	7	52.270	10.726	24.472	1.00	40.13	
ATOM	2737	OH2	TIP3	8	55.346	9.394	22.489	1.00	29.09	
ATOM	2740	OH2	TIP3	9	56.794	4.380	32.527	1.00	28.02	
ATOM	2743	OH2	TIP3	10	52.425	4.653	13.421	1.00	18.63	
ATOM	2746	OH2	TIP3	11	41.527	5.347	22.682	1.00	32.60	
ATOM	2749	OH2	TIP3	12	44.868	9.058	21.659	1.00	34.90	
ATOM	2752	OH2	TIP3	13	64.548	-2.881	29.048	1.00	32.56	
ATOM	2755	OH2	TIP3	14	77.179	13.205	23.892	1.00	30.36	
ATOM	2758	OH2	TIP3	15	79.309	16.826	18.132	1.00	55.69	
ATOM	2761	OH2	TIP3	16	83.279	11.681	16.069	1.00	21.18	
ATOM	2764	OH2	TIP3	17	13.978	-9.614	0.374	1.00	23.81	
ATOM	2767	OH2	TIP3	18	38.294	0.616	5.237	1.00	48.89	
ATOM	2770	OH2	TIP3	19	27.114	6.248	5.051	1.00	19.82	
ATOM	2773	OH2	TIP3	20	34.369	-1.759	16.798	1.00	43.83	
ATOM	2776	OH2	TIP3	21	20.500	2.296	28.237	1.00	53.46	
ATOM	2779	OH2	TIP3	22	50.938	-11.733	38.257	1.00	51.73	
ATOM	2782	OH2	TIP3	23	17.066	-5.917	-2.027	1.00	29.88	
ATOM	2785	OH2	TIP3	24	27.873	8.078	15.136	1.00	46.40	
ATOM	2788	OH2	TIP3	25	31.459	0.037	6.873	1.00	33.38	
ATOM	2791	OH2	TIP3	26	27.088	-12.845	27.724	1.00	37.01	
ATOM	2794	OH2	TIP3	27	28.577	-17.329	12.884	1.00	37.31	
ATOM	2797	OH2	TIP3	28	88.863	14.111	8.054	1.00	41.25	
ATOM	2800	OH2	TIP3	29	-2.311	-3.712	11.489	1.00	30.72	
ATOM	2803	OH2	TIP3	30	34.895	-4.269	18.658	1.00	28.99	
ATOM	2806	OH2	TIP3	31	80.531	18.007	9.739	1.00	23.83	
ATOM	2809	OH2	TIP3	32	5.519	3.787	10.628	1.00	20.39	
ATOM	2812	OH2	TIP3	33	-10.523	5.304	11.469	1.00	20.31	
ATOM	2815	OH2	TIP3	34	29.538	-8.848	20.187	1.00	43.26	
ATOM	2818	OH2	TIP3	35	5.866	3.469	13.367	1.00	21.16	
ATOM	2821	OH2	TIP3	36	31.810	3.038	0.203	1.00	65.03	
ATOM	2824	OH2	TIP3	37	19.879	2.087	-3.828	1.00	34.62	
ATOM	2827	OH2	TIP3	38	61.882	2.577	32.790	1.00	43.01	
ATOM	2830	OH2	TIP3	39	21.062	-6.897	-4.255	1.00	26.18	
ATOM	2833	OH2	TIP3	40	-15.562	8.847	22.744	1.00	40.33	
ATOM	2836	OH2	TIP3	41	40.043	2.380	8.610	1.00	65.14	
ATOM	2839	OH2	TIP3	42	19.176	11.322	0.332	1.00	33.04	
ATOM	2842	OH2	TIP3	43	67.221	8.965	17.535	1.00	14.78	
ATOM	2845	OH2	TIP3	44	87.877	18.828	18.789	1.00	50.00	
ATOM	2848	OH2	TIP3	45	74.676	17.083	4.253	1.00	43.45	
ATOM	2851	OH2	TIP3	46	29.458	16.709	10.527	1.00	37.44	
ATOM	2854	OH2	TIP3	47	66.590	7.242	15.359	1.00	27.63	
ATOM	2857	OH2	TIP3	48	85.038	21.651	5.881	1.00	27.12	
ATOM	2860	OH2	TIP3	49	-4.762	3.091	3.313	1.00	13.83	
ATOM	2863	OH2	TIP3	50	19.509	4.951	5.063	1.00	33.74	
ATOM	2866	OH2	TIP3	51	34.833	5.465	24.635	1.00	32.77	

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ATOM	2869	OH2 TIP3	52	34.907	-17.187	13.739	1.00	39.47
ATOM	2872	OH2 TIP3	53	60.000	7.568	27.982	1.00	31.38
ATOM	2875	OH2 TIP3	54	-7.341	-1.418	6.308	1.00	40.22
ATOM	2878	OH2 TIP3	55	55.218	12.161	25.430	1.00	40.99
ATOM	2881	OH2 TIP3	56	68.597	6.912	16.955	1.00	45.39
ATOM	2884	OH2 TIP3	57	73.486	20.957	19.260	1.00	49.23
ATOM	2887	OH2 TIP3	58	3.555	-8.367	-8.166	1.00	20.02
ATOM	2890	OH2 TIP3	59	38.079	10.933	5.669	1.00	27.07
ATOM	2893	OH2 TIP3	60	29.817	-9.690	-1.649	1.00	44.28
ATOM	2896	OH2 TIP3	61	49.332	1.501	12.262	1.00	42.78
ATOM	2899	OH2 TIP3	62	41.366	3.969	28.834	1.00	37.60
ATOM	2902	OH2 TIP3	63	10.523	-13.468	0.864	1.00	45.18
ATOM	2905	OH2 TIP3	64	-1.001	-4.658	21.574	1.00	35.58
ATOM	2908	OH2 TIP3	65	30.278	16.435	13.217	1.00	48.75
ATOM	2911	OH2 TIP3	66	8.115	4.304	3.317	1.00	16.04
ATOM	2914	OH2 TIP3	67	73.460	18.707	22.744	1.00	34.79
ATOM	2917	OH2 TIP3	68	-8.041	-3.332	24.939	1.00	44.96
ATOM	2920	OH2 TIP3	69	66.672	-4.643	28.739	1.00	62.39
ATOM	2923	OH2 TIP3	70	21.770	-20.943	4.990	1.00	32.98
ATOM	2926	OH2 TIP3	71	59.587	-6.482	5.018	1.00	37.78
ATOM	2929	OH2 TIP3	72	16.676	-13.158	-3.023	1.00	42.74
ATOM	2932	OH2 TIP3	73	-15.177	7.529	4.524	1.00	19.90
ATOM	2935	OH2 TIP3	74	33.105	2.738	13.267	1.00	40.43
ATOM	2938	OH2 TIP3	75	0.334	-2.795	10.999	1.00	31.20
ATOM	2941	OH2 TIP3	76	17.489	2.568	5.445	1.00	16.38
ATOM	2944	OH2 TIP3	77	27.373	3.870	6.168	1.00	39.52
ATOM	2947	OH2 TIP3	78	-8.546	6.378	9.673	1.00	17.89
ATOM	2950	OH2 TIP3	79	1.508	-1.891	8.809	1.00	33.71
ATOM	2953	OH2 TIP3	80	-4.985	-3.024	6.965	1.00	29.65
ATOM	2956	OH2 TIP3	81	17.673	3.019	1.736	1.00	22.73
ATOM	2959	OH2 TIP3	82	20.319	3.536	2.883	1.00	20.39
ATOM	2962	OH2 TIP3	83	0.366	-2.419	22.243	1.00	22.15
ATOM	2965	OH2 TIP3	84	19.688	-6.134	-1.678	1.00	13.22
ATOM	2968	OH2 TIP3	85	10.581	-15.481	6.681	1.00	43.14
ATOM	2971	OH2 TIP3	86	4.476	-12.368	11.861	1.00	38.38
ATOM	2974	OH2 TIP3	87	6.421	1.053	-3.368	1.00	21.50
ATOM	2977	OH2 TIP3	88	-13.766	1.683	5.565	1.00	39.45
ATOM	2980	OH2 TIP3	89	15.689	-7.291	-0.140	1.00	30.27
ATOM	2983	OH2 TIP3	90	-1.762	-5.389	3.937	1.00	31.03
ATOM	2986	OH2 TIP3	91	12.642	5.184	-4.424	1.00	37.94
ATOM	2989	OH2 TIP3	92	69.601	27.513	2.309	1.00	44.71
ATOM	2992	OH2 TIP3	93	24.342	-13.465	-0.010	1.00	50.74
ATOM	2995	OH2 TIP3	94	60.354	-4.675	33.978	1.00	38.15
ATOM	2998	OH2 TIP3	95	10.408	5.632	3.428	1.00	51.37
ATOM	3001	OH2 TIP3	96	-9.676	-3.916	4.621	1.00	34.12
ATOM	3004	OH2 TIP3	97	73.207	-2.076	10.677	1.00	70.04
ATOM	3007	OH2 TIP3	98	-3.042	5.487	30.579	1.00	30.78
ATOM	3010	OH2 TIP3	99	36.627	0.829	11.645	1.00	41.40
ATOM	3013	OH2 TIP3	100	21.685	6.318	16.814	1.00	20.93
ATOM	3016	OH2 TIP3	101	31.434	0.662	19.231	1.00	57.99
ATOM	3019	OH2 TIP3	102	5.793	-8.713	22.177	1.00	54.77
ATOM	3022	OH2 TIP3	103	-13.037	8.412	17.695	1.00	25.61

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ATOM	3025	OH2	TIP3	104	26.597	-10.647	-1.184	1.00	25.85
ATOM	3028	OH2	TIP3	105	24.406	1.951	18.037	1.00	30.72
ATOM	3031	OH2	TIP3	106	-1.809	12.914	3.754	1.00	43.57
ATOM	3034	OH2	TIP3	107	59.590	13.738	33.131	1.00	26.96
ATOM	3037	OH2	TIP3	108	4.442	-11.011	1.724	1.00	46.96
ATOM	3040	OH2	TIP3	109	8.101	2.869	0.801	1.00	37.28
ATOM	3043	OH2	TIP3	110	76.065	1.631	26.158	1.00	46.49
ATOM	3046	OH2	TIP3	111	48.821	15.839	14.239	1.00	34.18
ATOM	3049	OH2	TIP3	112	2.703	-11.324	8.959	1.00	39.16
ATOM	3052	OH2	TIP3	113	82.922	26.478	12.953	1.00	43.77
ATOM	3055	OH2	TIP3	114	8.998	-6.359	-3.309	1.00	39.51
ATOM	3058	OH2	TIP3	115	-8.590	4.563	4.397	1.00	32.53
ATOM	3061	OH2	TIP3	116	8.115	-13.800	8.351	1.00	41.64
ATOM	3064	OH2	TIP3	117	51.643	6.187	10.821	1.00	31.70
ATOM	3067	OH2	TIP3	118	20.737	3.915	15.522	1.00	17.40
ATOM	3070	OH2	TIP3	119	73.254	3.698	20.947	1.00	27.49
ATOM	3073	OH2	TIP3	120	5.343	-11.780	22.588	1.00	36.63
ATOM	3076	OH2	TIP3	121	34.390	2.307	16.660	1.00	64.04
ATOM	3079	OH2	TIP3	122	9.552	-11.846	6.934	1.00	28.23
ATOM	3082	OH2	TIP3	123	8.463	4.098	-1.454	1.00	30.21
ATOM	3085	OH2	TIP3	124	7.397	6.952	2.826	1.00	33.87
ATOM	3088	OH2	TIP3	125	35.796	-1.428	0.072	1.00	30.27
ATOM	3091	OH2	TIP3	126	45.044	10.052	11.102	1.00	28.75
ATOM	3094	OH2	TIP3	127	45.209	11.756	21.279	1.00	31.80
ATOM	3097	OH2	TIP3	128	-2.800	15.170	16.902	1.00	32.72
ATOM	3100	OH2	TIP3	129	85.885	11.248	9.428	1.00	25.28
ATOM	3103	OH2	TIP3	130	13.136	-2.420	1.867	1.00	20.56
ATOM	3106	OH2	TIP3	131	75.900	3.542	20.641	1.00	39.79
ATOM	3109	OH2	TIP3	132	13.075	7.580	-2.817	1.00	34.49
ATOM	3112	OH2	TIP3	133	11.166	-10.189	0.573	1.00	36.71
ATOM	3115	OH2	TIP3	134	13.814	-16.459	3.327	1.00	21.18
ATOM	3118	OH2	TIP3	135	-6.419	-3.460	16.599	1.00	32.62
ATOM	3121	OH2	TIP3	136	25.578	-12.834	3.624	1.00	43.32
ATOM	3124	OH2	TIP3	137	-16.472	11.136	6.388	1.00	64.77
ATOM	3127	OH2	TIP3	138	86.531	12.711	7.151	1.00	28.72
ATOM	3130	OH2	TIP3	139	32.292	-4.665	1.511	1.00	30.98
ATOM	3133	OH2	TIP3	140	45.116	7.369	11.774	1.00	30.59
ATOM	3136	OH2	TIP3	141	81.035	12.317	16.907	1.00	41.72
ATOM	3139	OH2	TIP3	142	2.905	-7.019	-2.101	1.00	26.20
ATOM	3142	OH2	TIP3	143	31.895	-6.253	20.885	1.00	36.12
ATOM	3145	OH2	TIP3	144	74.974	-2.640	12.464	1.00	58.90
ATOM	3148	OH2	TIP3	145	7.514	6.734	-1.116	1.00	37.81
ATOM	3151	OH2	TIP3	146	71.606	5.595	22.198	1.00	54.82
ATOM	3154	OH2	TIP3	147	68.337	-5.037	8.955	1.00	40.80
ATOM	3157	OH2	TIP3	148	0.191	-9.669	6.903	1.00	47.40
ATOM	3160	OH2	TIP3	149	68.043	18.153	10.710	1.00	36.67
ATOM	3163	OH2	TIP3	150	3.644	8.512	4.478	1.00	40.16
ATOM	3166	OH2	TIP3	151	52.117	11.302	18.644	1.00	40.22
ATOM	3169	OH2	TIP3	152	-10.220	6.750	4.981	1.00	25.00
ATOM	3172	OH2	TIP3	153	76.944	1.425	-0.793	1.00	46.95
ATOM	3175	OH2	TIP3	154	10.053	-11.958	17.014	1.00	38.99
ATOM	3178	OH2	TIP3	155	34.348	14.128	18.169	1.00	42.98

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ATOM	3181	OH2 TIP3	156	2.472	-8.230	16.629	1.00	39.28
ATOM	3184	OH2 TIP3	157	29.861	1.764	5.993	1.00	36.29
ATOM	3187	OH2 TIP3	158	32.608	-17.351	11.473	1.00	59.48
ATOM	3190	OH2 TIP3	159	42.408	18.047	11.188	1.00	39.61
ATOM	3193	OH2 TIP3	160	88.019	10.498	5.885	1.00	57.85
ATOM	3196	OH2 TIP3	161	70.091	-4.165	25.232	1.00	64.48
ATOM	3199	OH2 TIP3	162	77.332	5.434	24.000	1.00	55.68
ATOM	3202	OH2 TIP3	163	-0.743	-8.232	4.456	1.00	61.30
ATOM	3205	OH2 TIP3	164	34.224	15.617	1.556	1.00	36.76
ATOM	3208	OH2 TIP3	165	-9.619	7.593	7.404	1.00	36.55
ATOM	3211	OH2 TIP3	166	11.725	5.841	7.590	1.00	33.56
ATOM	3214	OH2 TIP3	167	-8.492	14.057	13.866	1.00	43.88
ATOM	3217	OH2 TIP3	168	32.082	3.374	18.430	1.00	50.87
ATOM	3220	OH2 TIP3	169	-8.471	9.925	24.255	1.00	41.24
ATOM	3223	OH2 TIP3	170	-1.100	-6.507	15.528	1.00	31.24
ATOM	3226	OH2 TIP3	171	80.411	0.680	15.823	1.00	49.76
ATOM	3229	OH2 TIP3	172	67.266	20.862	-1.548	1.00	43.71
ATOM	3232	OH2 TIP3	173	-0.460	4.230	1.362	1.00	29.46
ATOM	3235	OH2 TIP3	174	-0.107	6.721	2.716	1.00	34.57
ATOM	3238	OH2 TIP3	175	-0.955	8.958	1.388	1.00	37.76
ATOM	3241	OH2 TIP3	176	-5.269	9.229	2.243	1.00	38.77
ATOM	3244	OH2 TIP3	177	-7.000	10.196	3.928	1.00	55.41
ATOM	3247	OH2 TIP3	178	2.919	7.005	0.987	1.00	46.54
ATOM	3250	OH2 TIP3	179	5.370	10.843	8.420	1.00	36.98
ATOM	3253	OH2 TIP3	180	63.828	12.793	22.770	1.00	63.91
ATOM	3256	OH2 TIP3	181	79.461	0.958	18.507	1.00	47.46
ATOM	3259	OH2 TIP3	182	59.131	-11.907	7.222	1.00	51.47
ATOM	3262	OH2 TIP3	183	14.248	-1.085	-4.437	1.00	43.62
ATOM	3265	OH2 TIP3	184	59.294	2.993	33.283	1.00	56.42
ATOM	3268	OH2 TIP3	185	32.270	13.672	20.001	1.00	47.71
ATOM	3271	OH2 TIP3	186	72.089	16.139	22.904	1.00	49.99
ATOM	3274	OH2 TIP3	187	1.038	-8.592	14.174	1.00	40.01
ATOM	3277	OH2 TIP3	188	-0.484	5.267	30.679	1.00	48.08
ATOM	3280	OH2 TIP3	189	81.532	15.288	17.279	1.00	79.71
ATOM	3283	OH2 TIP3	190	-17.528	3.859	24.112	1.00	56.21
ATOM	3286	OH2 TIP3	191	27.542	10.591	14.666	1.00	53.58
ATOM	3289	OH2 TIP3	192	34.962	4.381	27.739	1.00	60.92
ATOM	3292	OH2 TIP3	193	-3.244	-3.943	8.937	1.00	35.88
ATOM	3295	OH2 TIP3	194	42.673	7.836	22.289	1.00	37.44
ATOM	3298	OH2 TIP3	195	52.865	12.074	22.272	1.00	35.63
ATOM	3301	OH2 TIP3	196	26.791	13.926	19.808	1.00	76.14
ATOM	3304	OH2 TIP3	197	-7.584	9.157	6.269	1.00	44.54
ATOM	3310	OH2 TIP3	198	55.298	15.955	20.455	1.00	50.69
ATOM	3313	OH2 TIP3	199	51.654	19.308	22.767	1.00	53.00
ATOM	3316	OH2 TIP3	200	20.092	7.039	7.056	1.00	32.98
ATOM	3319	OH2 TIP3	201	28.988	1.734	-3.437	1.00	42.52
ATOM	3322	OH2 TIP3	202	26.359	2.749	-4.689	1.00	43.12
ATOM	3325	OH2 TIP3	203	36.827	2.974	18.493	1.00	57.91
ATOM	3328	OH2 TIP3	204	17.012	-20.743	13.983	1.00	62.01
ATOM	3331	OH2 TIP3	205	27.980	-14.283	6.114	1.00	79.57
ATOM	3334	OH2 TIP3	206	31.396	1.595	-1.941	1.00	53.29
ATOM	3337	OH2 TIP3	207	10.244	-16.264	15.463	1.00	43.25

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ATOM	3340	OH2	TIP3	208	7.255	-11.909	5.440	1.00	45.52
ATOM	3343	OH2	TIP3	209	-12.421	14.520	11.103	1.00	56.32
ATOM	3346	OH2	TIP3	210	11.250	9.879	-1.498	1.00	28.34
ATOM	3349	OH2	TIP3	211	11.426	12.574	-1.341	1.00	37.79
ATOM	3352	OH2	TIP3	212	34.344	13.104	-1.291	1.00	51.83
ATOM	3355	OH2	TIP3	213	31.230	18.082	8.054	1.00	44.77
ATOM	3358	OH2	TIP3	214	37.062	12.036	-1.875	1.00	53.61
ATOM	3361	OH2	TIP3	215	35.231	3.150	10.692	1.00	60.59
ATOM	3364	OH2	TIP3	216	63.913	13.371	26.770	1.00	59.44
ATOM	3367	OH2	TIP3	217	36.511	6.165	15.409	1.00	70.98
ATOM	3370	OH2	TIP3	218	90.623	4.459	6.671	1.00	52.23
ATOM	3373	OH2	TIP3	219	49.822	-11.758	10.881	1.00	46.12
ATOM	3376	OH2	TIP3	220	60.367	-10.286	16.662	1.00	68.41
ATOM	3379	OH2	TIP3	221	17.954	-21.378	7.048	1.00	68.51
ATOM	3382	OH2	TIP3	222	66.176	-1.266	30.784	1.00	39.19
ATOM	3385	OH2	TIP3	223	75.201	19.402	20.800	1.00	43.98
ATOM	3388	OH2	TIP3	224	-2.895	10.302	3.534	1.00	44.97
ATOM	3391	OH2	TIP3	225	6.045	-4.015	25.279	1.00	63.74
ATOM	3394	OH2	TIP3	226	36.238	5.898	12.819	1.00	32.89
ATOM	3397	OH2	TIP3	227	-5.516	16.713	14.089	1.00	51.60
ATOM	3400	OH2	TIP3	228	46.577	-11.931	26.964	1.00	37.76
ATOM	3403	OH2	TIP3	229	6.496	6.048	13.722	1.00	27.51
ATOM	3406	OH2	TIP3	230	-3.691	-5.054	20.691	1.00	38.16
ATOM	3409	OH2	TIP3	231	1.811	-3.444	-0.149	1.00	54.03
ATOM	3412	OH2	TIP3	232	86.148	11.480	23.402	1.00	57.66
ATOM	3415	OH2	TIP3	233	10.549	7.581	5.716	1.00	48.49
ATOM	3421	OH2	TIP3	234	64.680	-8.130	20.697	1.00	69.67
ATOM	3424	OH2	TIP3	235	11.380	-17.736	13.500	1.00	54.61
ATOM	3427	OH2	TIP3	236	3.136	-4.782	21.980	1.00	57.12
ATOM	3430	OH2	TIP3	237	72.296	1.006	-1.987	1.00	41.40
ATOM	3433	OH2	TIP3	238	50.258	-3.179	32.723	1.00	74.99
ATOM	3436	OH2	TIP3	239	58.051	9.469	11.776	1.00	44.10
ATOM	3439	OH2	TIP3	240	43.530	20.498	30.344	1.00	43.69
ATOM	3442	OH2	TIP3	241	67.081	16.597	15.934	1.00	45.80
ATOM	3445	OH2	TIP3	242	87.660	21.694	5.373	1.00	50.39
ATOM	3448	OH2	TIP3	243	71.779	28.586	7.932	1.00	61.12
ATOM	3451	OH2	TIP3	244	25.965	-8.124	27.084	1.00	42.13
ATOM	3454	OH2	TIP3	245	-18.336	10.487	12.859	1.00	73.36
ATOM	3457	OH2	TIP3	246	30.703	11.410	16.381	1.00	39.24
ATOM	3460	OH2	TIP3	247	22.617	-16.025	-2.906	1.00	63.22
ATOM	4620	C	SUG	1000	67.815	4.441	11.493	1.00	20.00
ATOM	4621	C1	SUG	1000	67.387	3.706	10.364	1.00	20.00
ATOM	4622	N	SUG	1000	67.823	2.445	9.937	1.00	20.00
ATOM	4623	C2	SUG	1000	66.401	4.224	9.501	1.00	20.00
ATOM	4624	C3	SUG	1000	65.825	5.499	9.765	1.00	20.00
ATOM	4625	C4	SUG	1000	66.259	6.212	10.884	1.00	20.00
ATOM	4626	C5	SUG	1000	67.239	5.690	11.736	1.00	20.00
ATOM	4627	C6	SUG	1000	66.155	3.220	8.401	1.00	20.00
ATOM	4628	O	SUG	1000	67.372	1.047	8.275	1.00	20.00
ATOM	4629	C7	SUG	1000	67.155	2.121	8.828	1.00	20.00
ATOM	4630	C8	SUG	1000	63.369	2.460	5.852	1.00	20.00
ATOM	4631	C9	SUG	1000	65.284	3.356	7.382	1.00	20.00

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ATOM	4632	C10	SUG	1000	64.603	2.300	6.514	1.00	20.00
ATOM	4633	C11	SUG	1000	64.167	0.392	5.481	1.00	20.00
ATOM	4634	C12	SUG	1000	63.106	1.251	5.206	1.00	20.00
ATOM	4635	N13	SUG	1000	65.103	1.023	6.293	1.00	20.00
ATOM	4636	C14	SUG	1000	61.898	0.897	4.346	1.00	20.00
ATOM	4637	C15	SUG	1000	62.476	3.715	5.826	1.00	20.00
ATOM	4638	C16	SUG	1000	61.259	3.598	6.771	1.00	20.00
ATOM	4639	O1	SUG	1000	60.814	5.963	6.429	1.00	20.00
ATOM	4640	C17	SUG	1000	60.520	4.912	6.988	1.00	20.00
ATOM	4641	O2	SUG	1000	59.496	4.795	7.873	1.00	20.00
ATOM	4642	C	SUG	1001	5.413	2.967	18.087	1.00	20.00
ATOM	4643	C1	SUG	1001	5.891	2.927	19.417	1.00	20.00
ATOM	4644	N	SUG	1001	5.553	2.021	20.431	1.00	20.00
ATOM	4645	C2	SUG	1001	6.828	3.875	19.872	1.00	20.00
ATOM	4646	C3	SUG	1001	7.304	4.884	18.988	1.00	20.00
ATOM	4647	C4	SUG	1001	6.822	4.909	17.678	1.00	20.00
ATOM	4648	C5	SUG	1001	5.890	3.964	17.233	1.00	20.00
ATOM	4649	C6	SUG	1001	7.145	3.576	21.318	1.00	20.00
ATOM	4650	O	SUG	1001	6.101	1.678	22.552	1.00	20.00
ATOM	4651	C7	SUG	1001	6.237	2.343	21.530	1.00	20.00
ATOM	4652	C8	SUG	1001	9.967	4.392	23.809	1.00	20.00
ATOM	4653	C9	SUG	1001	7.997	4.264	22.102	1.00	20.00
ATOM	4654	C10	SUG	1001	8.753	3.835	23.357	1.00	20.00
ATOM	4655	C11	SUG	1001	9.331	2.736	25.189	1.00	20.00
ATOM	4656	C12	SUG	1001	10.320	3.689	24.962	1.00	20.00
ATOM	4657	N13	SUG	1001	8.354	2.808	24.203	1.00	20.00
ATOM	4658	C14	SUG	1001	11.547	3.900	25.843	1.00	20.00
ATOM	4659	C15	SUG	1001	10.759	5.550	23.175	1.00	20.00
ATOM	4660	C16	SUG	1001	11.987	5.063	22.373	1.00	20.00
ATOM	4661	O1	SUG	1001	12.243	7.308	21.475	1.00	20.00
ATOM	4662	C17	SUG	1001	12.621	6.142	21.504	1.00	20.00
ATOM	4663	O2	SUG	1001	13.657	5.670	20.762	1.00	20.00

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TABLE 4

Atom No.	Atom Type	A.A Type	A.A No.	X	Y	Z	OCC	B
ATOM	1	N	GLU	1464	-13.576	17.066	8.598	1.00 57.39
ATOM	2	CA	GLU	1464	-12.446	17.198	7.684	1.00 55.83
ATOM	3	CB	GLU	1464	-11.381	18.127	8.275	1.00 56.73
ATOM	4	C	GLU	1464	-11.845	15.833	7.341	1.00 55.07
ATOM	5	O	GLU	1464	-11.722	15.504	6.165	1.00 59.74
ATOM	6	N	LEU	1465	-11.518	15.023	8.347	1.00 50.12
ATOM	7	CA	LEU	1465	-10.950	13.699	8.087	1.00 44.43
ATOM	8	CB	LEU	1465	-10.155	13.196	9.291	1.00 43.28
ATOM	9	CG	LEU	1465	-8.630	13.316	9.227	1.00 43.70
ATOM	10	CD1	LEU	1465	-8.222	14.754	9.013	1.00 47.59
ATOM	11	CD2	LEU	1465	-8.017	12.803	10.506	1.00 42.63
ATOM	12	C	LEU	1465	-12.046	12.697	7.739	1.00 40.93
ATOM	13	O	LEU	1465	-13.139	12.730	8.301	1.00 39.13
ATOM	14	N	PRO	1466	-11.794	11.852	6.726	1.00 40.49
ATOM	15	CD	PRO	1466	-10.612	11.884	5.844	1.00 39.07
ATOM	16	CA	PRO	1466	-12.754	10.831	6.284	1.00 40.14
ATOM	17	CB	PRO	1466	-12.152	10.331	4.981	1.00 40.90
ATOM	18	CG	PRO	1466	-10.664	10.518	5.202	1.00 41.39
ATOM	19	C	PRO	1466	-12.862	9.701	7.305	1.00 40.06
ATOM	20	O	PRO	1466	-11.857	9.290	7.883	1.00 40.71
ATOM	21	N	GLU	1467	-14.064	9.175	7.491	1.00 38.65
ATOM	22	CA	GLU	1467	-14.255	8.126	8.467	1.00 39.24
ATOM	23	CB	GLU	1467	-15.722	8.054	8.873	1.00 45.06
ATOM	24	CG	GLU	1467	-16.314	9.365	9.353	1.00 50.91
ATOM	25	CD	GLU	1467	-17.789	9.252	9.699	1.00 53.51
ATOM	26	OE1	GLU	1467	-18.379	8.170	9.504	1.00 54.15
ATOM	27	OE2	GLU	1467	-18.369	10.250	10.160	1.00 53.10
ATOM	28	C	GLU	1467	-13.808	6.777	7.914	1.00 36.09
ATOM	29	O	GLU	1467	-13.922	6.529	6.711	1.00 38.58
ATOM	30	N	ASP	1468	-13.272	5.929	8.791	1.00 30.71
ATOM	31	CA	ASP	1468	-12.839	4.592	8.407	1.00 28.23
ATOM	32	CB	ASP	1468	-11.328	4.515	8.186	1.00 25.51
ATOM	33	CG	ASP	1468	-10.885	3.207	7.529	1.00 27.68
ATOM	34	OD1	ASP	1468	-11.623	2.199	7.572	1.00 26.01
ATOM	35	OD2	ASP	1468	-9.777	3.187	6.962	1.00 28.87
ATOM	36	C	ASP	1468	-13.274	3.627	9.493	1.00 27.74
ATOM	37	O	ASP	1468	-12.570	3.405	10.493	1.00 25.83
ATOM	38	N	PRO	1469	-14.450	3.019	9.305	1.00 25.88
ATOM	39	CD	PRO	1469	-15.396	3.175	8.183	1.00 24.25
ATOM	40	CA	PRO	1469	-14.963	2.079	10.294	1.00 26.69
ATOM	41	CB	PRO	1469	-16.255	1.586	9.641	1.00 28.81
ATOM	42	CG	PRO	1469	-16.702	2.776	8.816	1.00 24.20
ATOM	43	C	PRO	1469	-14.012	0.925	10.625	1.00 27.51
ATOM	44	O	PRO	1469	-14.172	0.285	11.657	1.00 27.60
ATOM	45	N	ARG	1470	-13.075	0.642	9.720	1.00 26.49
ATOM	46	CA	ARG	1470	-12.108	-0.435	9.935	1.00 27.60

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ATOM	47	CB	ARG	1470	-11.285	-0.691	8.668	1.00	26.08
ATOM	48	CG	ARG	1470	-12.073	-1.125	7.439	1.00	30.77
ATOM	49	CD	ARG	1470	-11.153	-1.257	6.213	1.00	31.66
ATOM	50	NE	ARG	1470	-10.462	0.001	5.915	1.00	30.94
ATOM	51	CZ	ARG	1470	-9.577	0.167	4.941	1.00	33.30
ATOM	52	NH1	ARG	1470	-9.249	-0.846	4.144	1.00	32.78
ATOM	53	NH2	ARG	1470	-8.990	1.346	4.779	1.00	27.16
ATOM	54	C	ARG	1470	-11.116	-0.163	11.069	1.00	28.73
ATOM	55	O	ARG	1470	-10.588	-1.091	11.673	1.00	27.30
ATOM	56	N	TRP	1471	-10.871	1.107	11.363	1.00	27.98
ATOM	57	CA	TRP	1471	-9.892	1.430	12.375	1.00	26.33
ATOM	58	CB	TRP	1471	-8.642	1.964	11.671	1.00	23.87
ATOM	59	CG	TRP	1471	-7.998	0.947	10.795	1.00	24.61
ATOM	60	CD2	TRP	1471	-7.110	-0.104	11.205	1.00	23.32
ATOM	61	CE2	TRP	1471	-6.732	-0.807	10.041	1.00	24.34
ATOM	62	CE3	TRP	1471	-6.589	-0.509	12.438	1.00	21.39
ATOM	63	CD1	TRP	1471	-8.129	0.831	9.446	1.00	25.07
ATOM	64	NE1	TRP	1471	-7.369	-0.220	8.980	1.00	26.82
ATOM	65	CZ2	TRP	1471	-5.860	-1.898	10.083	1.00	23.12
ATOM	66	CZ3	TRP	1471	-5.722	-1.589	12.473	1.00	21.02
ATOM	67	CH2	TRP	1471	-5.364	-2.265	11.306	1.00	21.74
ATOM	68	C	TRP	1471	-10.292	2.384	13.478	1.00	26.93
ATOM	69	O	TRP	1471	-9.551	2.544	14.452	1.00	26.37
ATOM	70	N	GLU	1472	-11.464	2.975	13.364	1.00	26.40
ATOM	71	CA	GLU	1472	-11.909	3.959	14.341	1.00	27.12
ATOM	72	CB	GLU	1472	-13.168	4.674	13.821	1.00	28.25
ATOM	73	CG	GLU	1472	-13.497	6.026	14.498	1.00	27.47
ATOM	74	CD	GLU	1472	-12.611	7.180	14.042	1.00	24.64
ATOM	75	OE1	GLU	1472	-11.877	7.038	13.042	1.00	24.60
ATOM	76	OE2	GLU	1472	-12.658	8.247	14.683	1.00	23.70
ATOM	77	C	GLU	1472	-12.179	3.421	15.735	1.00	25.89
ATOM	78	O	GLU	1472	-12.795	2.373	15.891	1.00	27.74
ATOM	79	N	LEU	1473	-11.689	4.121	16.745	1.00	25.95
ATOM	80	CA	LEU	1473	-11.961	3.740	18.129	1.00	27.45
ATOM	81	CB	LEU	1473	-10.707	3.311	18.890	1.00	24.99
ATOM	82	CG	LEU	1473	-10.958	3.090	20.392	1.00	21.80
ATOM	83	CD1	LEU	1473	-11.551	1.696	20.627	1.00	20.63
ATOM	84	CD2	LEU	1473	-9.646	3.199	21.157	1.00	22.34
ATOM	85	C	LEU	1473	-12.478	5.008	18.752	1.00	29.33
ATOM	86	O	LEU	1473	-12.007	6.101	18.405	1.00	27.56
ATOM	87	N	PRO	1474	-13.529	4.896	19.585	1.00	30.07
ATOM	88	CD	PRO	1474	-14.380	3.704	19.737	1.00	29.18
ATOM	89	CA	PRO	1474	-14.124	6.051	20.267	1.00	29.03
ATOM	90	CB	PRO	1474	-15.266	5.406	21.062	1.00	26.83
ATOM	91	CG	PRO	1474	-15.701	4.307	20.158	1.00	26.35
ATOM	92	C	PRO	1474	-13.099	6.715	21.178	1.00	31.01
ATOM	93	O	PRO	1474	-12.310	6.042	21.850	1.00	33.14
ATOM	94	N	ARG	1475	-13.110	8.038	21.178	1.00	31.33
ATOM	95	CA	ARG	1475	-12.181	8.810	21.973	1.00	32.99
ATOM	96	CB	ARG	1475	-12.442	10.292	21.791	1.00	35.87
ATOM	97	CG	ARG	1475	-12.082	10.729	20.413	1.00	43.88
ATOM	98	CD	ARG	1475	-11.984	12.228	20.247	1.00	44.84

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ATOM	99	NE	ARG	1475	-11.665	12.499	18.846	1.00	48.59
ATOM	100	CZ	ARG	1475	-10.435	12.663	18.374	1.00	46.00
ATOM	101	NH1	ARG	1475	-9.400	12.618	19.202	1.00	46.56
ATOM	102	NH2	ARG	1475	-10.241	12.746	17.065	1.00	44.18
ATOM	103	C	ARG	1475	-12.175	8.456	23.442	1.00	35.47
ATOM	104	O	ARG	1475	-11.115	8.400	24.072	1.00	37.44
ATOM	105	N	ASP	1476	-13.347	8.134	23.974	1.00	35.04
ATOM	106	CA	ASP	1476	-13.468	7.800	25.380	1.00	34.30
ATOM	107	CB	ASP	1476	-14.940	7.853	25.797	1.00	36.89
ATOM	108	CG	ASP	1476	-15.796	6.818	25.089	1.00	38.67
ATOM	109	OD1	ASP	1476	-15.288	6.056	24.234	1.00	41.19
ATOM	110	OD2	ASP	1476	-16.995	6.758	25.406	1.00	48.08
ATOM	111	C	ASP	1476	-12.858	6.457	25.770	1.00	33.67
ATOM	112	O	ASP	1476	-12.830	6.109	26.949	1.00	36.57
ATOM	113	N	ARG	1477	-12.441	5.670	24.781	1.00	32.72
ATOM	114	CA	ARG	1477	-11.828	4.370	25.033	1.00	29.68
ATOM	115	CB	ARG	1477	-12.117	3.418	23.886	1.00	25.53
ATOM	116	CG	ARG	1477	-13.564	3.189	23.599	1.00	23.83
ATOM	117	CD	ARG	1477	-14.234	2.525	24.772	1.00	26.80
ATOM	118	NE	ARG	1477	-14.493	3.485	25.842	1.00	27.24
ATOM	119	CZ	ARG	1477	-14.818	3.145	27.085	1.00	27.41
ATOM	120	NH1	ARG	1477	-14.931	1.874	27.438	1.00	29.00
ATOM	121	NH2	ARG	1477	-15.005	4.095	27.985	1.00	25.85
ATOM	122	C	ARG	1477	-10.316	4.489	25.177	1.00	30.44
ATOM	123	O	ARG	1477	-9.616	3.515	25.461	1.00	32.78
ATOM	124	N	LEU	1478	-9.800	5.690	25.002	1.00	30.39
ATOM	125	CA	LEU	1478	-8.370	5.883	25.080	1.00	31.96
ATOM	126	CB	LEU	1478	-7.886	6.508	23.771	1.00	30.43
ATOM	127	CG	LEU	1478	-6.400	6.424	23.431	1.00	31.90
ATOM	128	CD1	LEU	1478	-5.939	4.964	23.382	1.00	28.92
ATOM	129	CD2	LEU	1478	-6.159	7.115	22.102	1.00	33.55
ATOM	130	C	LEU	1478	-7.974	6.757	26.265	1.00	33.60
ATOM	131	O	LEU	1478	-8.193	7.972	26.251	1.00	33.96
ATOM	132	N	VAL	1479	-7.416	6.140	27.305	1.00	33.54
ATOM	133	CA	VAL	1479	-6.974	6.902	28.468	1.00	32.52
ATOM	134	CB	VAL	1479	-7.085	6.089	29.757	1.00	32.76
ATOM	135	CG1	VAL	1479	-6.728	6.973	30.926	1.00	33.27
ATOM	136	CG2	VAL	1479	-8.493	5.537	29.913	1.00	30.15
ATOM	137	C	VAL	1479	-5.529	7.341	28.239	1.00	34.24
ATOM	138	O	VAL	1479	-4.581	6.546	28.350	1.00	32.24
ATOM	139	N	LEU	1480	-5.381	8.607	27.867	1.00	35.88
ATOM	140	CA	LEU	1480	-4.077	9.192	27.569	1.00	38.43
ATOM	141	CB	LEU	1480	-4.241	10.541	26.855	1.00	36.93
ATOM	142	CG	LEU	1480	-4.828	10.535	25.435	1.00	35.67
ATOM	143	CD1	LEU	1480	-4.762	11.952	24.907	1.00	32.47
ATOM	144	CD2	LEU	1480	-4.037	9.613	24.499	1.00	33.60
ATOM	145	C	LEU	1480	-3.144	9.324	28.768	1.00	39.70
ATOM	146	O	LEU	1480	-3.511	9.912	29.784	1.00	39.88
ATOM	147	N	GLY	1481	-1.912	8.842	28.610	1.00	39.70
ATOM	148	CA	GLY	1481	-0.960	8.896	29.700	1.00	41.31
ATOM	149	C	GLY	1481	0.349	9.633	29.474	1.00	44.39
ATOM	150	O	GLY	1481	0.429	10.626	28.744	1.00	45.69

ATOM	151	N	LYS	1482	1.389	9.122	30.124	1.00	44.73
ATOM	152	CA	LYS	1482	2.728	9.700	30.069	1.00	46.91
ATOM	153	CB	LYS	1482	3.649	8.934	31.023	1.00	51.20
ATOM	154	CG	LYS	1482	5.135	9.056	30.744	1.00	57.10
ATOM	155	CD	LYS	1482	5.878	7.826	31.248	1.00	60.81
ATOM	156	CE	LYS	1482	5.430	6.567	30.515	1.00	61.24
ATOM	157	NZ	LYS	1482	6.235	5.375	30.912	1.00	65.39
ATOM	158	C	LYS	1482	3.370	9.782	28.681	1.00	46.09
ATOM	159	O	LYS	1482	3.440	8.782	27.944	1.00	42.98
ATOM	160	N	PRO	1483	3.886	10.969	28.324	1.00	46.65
ATOM	161	CD	PRO	1483	3.910	12.184	29.152	1.00	46.11
ATOM	162	CA	PRO	1483	4.536	11.212	27.036	1.00	45.96
ATOM	163	CB	PRO	1483	5.015	12.660	27.172	1.00	43.59
ATOM	164	CG	PRO	1483	4.041	13.253	28.122	1.00	45.37
ATOM	165	C	PRO	1483	5.739	10.279	26.912	1.00	46.43
ATOM	166	O	PRO	1483	6.506	10.139	27.861	1.00	44.77
ATOM	167	N	LEU	1484	5.844	9.579	25.786	1.00	48.21
ATOM	168	CA	LEU	1484	6.978	8.684	25.554	1.00	50.46
ATOM	169	CB	LEU	1484	6.543	7.426	24.811	1.00	49.38
ATOM	170	CG	LEU	1484	5.655	6.437	25.576	1.00	50.15
ATOM	171	CD1	LEU	1484	5.067	5.422	24.615	1.00	44.90
ATOM	172	CD2	LEU	1484	6.446	5.750	26.669	1.00	44.60
ATOM	173	C	LEU	1484	8.058	9.419	24.764	1.00	53.33
ATOM	174	O	LEU	1484	9.241	9.116	24.896	1.00	51.94
ATOM	175	N	GLY	1485	7.643	10.376	23.931	1.00	57.68
ATOM	176	CA	GLY	1485	8.603	11.140	23.148	1.00	60.27
ATOM	177	C	GLY	1485	7.997	11.946	22.016	1.00	62.66
ATOM	178	O	GLY	1485	6.774	12.090	21.924	1.00	64.91
ATOM	179	N	GLN	1491	4.704	14.425	18.904	1.00	47.86
ATOM	180	CA	GLN	1491	4.339	13.868	20.206	1.00	44.42
ATOM	181	CB	GLN	1491	3.373	14.829	20.918	1.00	44.31
ATOM	182	C	GLN	1491	3.755	12.433	20.170	1.00	43.09
ATOM	183	O	GLN	1491	2.807	12.150	19.426	1.00	43.67
ATOM	184	N	VAL	1492	4.338	11.542	20.974	1.00	40.40
ATOM	185	CA	VAL	1492	3.903	10.143	21.101	1.00	39.95
ATOM	186	CB	VAL	1492	4.962	9.119	20.673	1.00	37.64
ATOM	187	CG1	VAL	1492	4.416	7.721	20.897	1.00	34.94
ATOM	188	CG2	VAL	1492	5.336	9.296	19.233	1.00	40.26
ATOM	189	C	VAL	1492	3.720	9.905	22.586	1.00	40.23
ATOM	190	O	VAL	1492	4.679	10.038	23.355	1.00	40.41
ATOM	191	N	VAL	1493	2.516	9.518	22.993	1.00	38.15
ATOM	192	CA	VAL	1493	2.250	9.291	24.405	1.00	37.11
ATOM	193	CB	VAL	1493	1.131	10.245	24.924	1.00	37.83
ATOM	194	CG1	VAL	1493	1.386	11.656	24.422	1.00	36.45
ATOM	195	CG2	VAL	1493	-0.252	9.769	24.508	1.00	39.28
ATOM	196	C	VAL	1493	1.854	7.844	24.701	1.00	36.02
ATOM	197	O	VAL	1493	1.450	7.118	23.797	1.00	37.17
ATOM	198	N	LEU	1494	2.052	7.418	25.944	1.00	32.77
ATOM	199	CA	LEU	1494	1.645	6.081	26.335	1.00	30.87
ATOM	200	CB	LEU	1494	2.445	5.587	27.550	1.00	27.22
ATOM	201	CG	LEU	1494	1.970	4.250	28.141	1.00	28.67
ATOM	202	CD1	LEU	1494	2.124	3.132	27.129	1.00	27.40

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ATOM	203	CD2	LEU	1494	2.736	3.904	29.377	1.00	28.84
ATOM	204	C	LEU	1494	0.173	6.256	26.701	1.00	31.18
ATOM	205	O	LEU	1494	-0.249	7.344	27.119	1.00	30.88
ATOM	206	N	ALA	1495	-0.626	5.223	26.477	1.00	30.40
ATOM	207	CA	ALA	1495	-2.044	5.307	26.817	1.00	28.30
ATOM	208	CB	ALA	1495	-2.815	5.999	25.691	1.00	27.35
ATOM	209	C	ALA	1495	-2.608	3.919	27.057	1.00	26.32
ATOM	210	O	ALA	1495	-1.926	2.915	26.846	1.00	24.54
ATOM	211	N	GLU	1496	-3.836	3.867	27.552	1.00	28.11
ATOM	212	CA	GLU	1496	-4.514	2.603	27.793	1.00	29.22
ATOM	213	CB	GLU	1496	-4.841	2.441	29.272	1.00	31.77
ATOM	214	CG	GLU	1496	-3.627	2.233	30.140	1.00	37.26
ATOM	215	CD	GLU	1496	-3.950	2.405	31.613	1.00	39.77
ATOM	216	OE1	GLU	1496	-4.322	3.534	31.999	1.00	37.54
ATOM	217	OE2	GLU	1496	-3.835	1.417	32.378	1.00	41.52
ATOM	218	C	GLU	1496	-5.799	2.594	26.970	1.00	29.76
ATOM	219	O	GLU	1496	-6.593	3.543	27.020	1.00	31.39
ATOM	220	N	ALA	1497	-5.961	1.561	26.153	1.00	29.55
ATOM	221	CA	ALA	1497	-7.139	1.426	25.324	1.00	28.69
ATOM	222	CB	ALA	1497	-6.742	0.969	23.930	1.00	23.86
ATOM	223	C	ALA	1497	-8.068	0.418	25.965	1.00	29.51
ATOM	224	O	ALA	1497	-7.657	-0.702	26.278	1.00	30.40
ATOM	225	N	ILE	1498	-9.313	0.823	26.201	1.00	31.33
ATOM	226	CA	ILE	1498	-10.302	-0.064	26.811	1.00	32.30
ATOM	227	CB	ILE	1498	-11.359	0.727	27.619	1.00	33.61
ATOM	228	CG2	ILE	1498	-12.233	-0.246	28.439	1.00	34.55
ATOM	229	CG1	ILE	1498	-10.690	1.745	28.545	1.00	31.99
ATOM	230	CD1	ILE	1498	-11.663	2.730	29.155	1.00	26.68
ATOM	231	C	ILE	1498	-11.023	-0.777	25.673	1.00	32.69
ATOM	232	O	ILE	1498	-11.644	-0.134	24.838	1.00	32.03
ATOM	233	N	GLY	1499	-10.917	-2.095	25.610	1.00	37.34
ATOM	234	CA	GLY	1499	-11.588	-2.822	24.554	1.00	44.45
ATOM	235	C	GLY	1499	-10.709	-3.193	23.372	1.00	50.75
ATOM	236	O	GLY	1499	-9.993	-4.205	23.438	1.00	53.68
ATOM	237	N	LEU	1500	-10.729	-2.370	22.321	1.00	51.14
ATOM	238	CA	LEU	1500	-9.963	-2.613	21.087	1.00	51.15
ATOM	239	CB	LEU	1500	-8.445	-2.677	21.345	1.00	50.85
ATOM	240	CG	LEU	1500	-7.516	-1.463	21.166	1.00	49.05
ATOM	241	CD1	LEU	1500	-6.082	-1.946	21.263	1.00	44.92
ATOM	242	CD2	LEU	1500	-7.703	-0.783	19.824	1.00	44.03
ATOM	243	C	LEU	1500	-10.420	-3.891	20.376	1.00	50.50
ATOM	244	O	LEU	1500	-10.544	-4.966	20.984	1.00	49.92
ATOM	245	N	PRO	1505	-13.321	-5.777	25.373	1.00	48.57
ATOM	246	CD	PRO	1505	-13.937	-7.111	25.286	1.00	50.09
ATOM	247	CA	PRO	1505	-14.289	-4.776	25.848	1.00	46.31
ATOM	248	CB	PRO	1505	-15.630	-5.503	25.710	1.00	45.25
ATOM	249	CG	PRO	1505	-15.271	-6.918	26.025	1.00	48.85
ATOM	250	C	PRO	1505	-14.010	-4.321	27.294	1.00	43.31
ATOM	251	O	PRO	1505	-14.001	-3.122	27.571	1.00	42.84
ATOM	252	N	ASN	1506	-13.712	-5.272	28.178	1.00	40.46
ATOM	253	CA	ASN	1506	-13.430	-4.945	29.571	1.00	42.33
ATOM	254	CB	ASN	1506	-14.302	-5.776	30.512	1.00	43.55

ATOM	255	CG	ASN	1506	-15.760	-5.436	30.382	1.00	42.68
ATOM	256	OD1	ASN	1506	-16.141	-4.269	30.316	1.00	47.11
ATOM	257	ND2	ASN	1506	-16.591	-6.461	30.323	1.00	45.66
ATOM	258	C	ASN	1506	-11.962	-5.097	29.957	1.00	42.89
ATOM	259	O	ASN	1506	-11.617	-5.221	31.137	1.00	43.23
ATOM	260	N	ARG	1507	-11.099	-5.066	28.949	1.00	42.72
ATOM	261	CA	ARG	1507	-9.661	-5.186	29.145	1.00	42.24
ATOM	262	CB	ARG	1507	-9.144	-6.384	28.353	1.00	50.39
ATOM	263	CG	ARG	1507	-9.407	-7.728	28.992	1.00	60.88
ATOM	264	CD	ARG	1507	-8.357	-8.063	30.038	1.00	67.47
ATOM	265	NE	ARG	1507	-8.566	-9.401	30.574	1.00	74.19
ATOM	266	CZ	ARG	1507	-8.012	-9.861	31.691	1.00	79.97
ATOM	267	NH1	ARG	1507	-7.193	-9.093	32.406	1.00	81.67
ATOM	268	NH2	ARG	1507	-8.338	-11.068	32.134	1.00	82.38
ATOM	269	C	ARG	1507	-8.982	-3.940	28.611	1.00	38.15
ATOM	270	O	ARG	1507	-9.458	-3.354	27.642	1.00	36.46
ATOM	271	N	VAL	1508	-7.927	-3.491	29.279	1.00	35.19
ATOM	272	CA	VAL	1508	-7.190	-2.335	28.782	1.00	33.82
ATOM	273	CB	VAL	1508	-6.824	-1.296	29.883	1.00	30.19
ATOM	274	CG1	VAL	1508	-8.072	-0.723	30.498	1.00	34.68
ATOM	275	CG2	VAL	1508	-5.948	-1.900	30.938	1.00	28.53
ATOM	276	C	VAL	1508	-5.912	-2.869	28.155	1.00	33.91
ATOM	277	O	VAL	1508	-5.392	-3.926	28.555	1.00	34.02
ATOM	278	N	THR	1509	-5.427	-2.152	27.154	1.00	31.32
ATOM	279	CA	THR	1509	-4.206	-2.527	26.476	1.00	30.47
ATOM	280	CB	THR	1509	-4.492	-3.015	25.031	1.00	30.88
ATOM	281	OG1	THR	1509	-5.522	-4.008	25.066	1.00	33.90
ATOM	282	CG2	THR	1509	-3.255	-3.648	24.411	1.00	24.49
ATOM	283	C	THR	1509	-3.323	-1.300	26.419	1.00	28.74
ATOM	284	O	THR	1509	-3.774	-0.219	26.039	1.00	27.29
ATOM	285	N	LYS	1510	-2.092	-1.432	26.893	1.00	29.17
ATOM	286	CA	LYS	1510	-1.162	-0.325	26.831	1.00	30.55
ATOM	287	CB	LYS	1510	0.092	-0.595	27.648	1.00	27.23
ATOM	288	CG	LYS	1510	-0.117	-0.460	29.135	1.00	34.33
ATOM	289	CD	LYS	1510	1.191	-0.614	29.896	1.00	40.49
ATOM	290	CE	LYS	1510	1.065	-1.603	31.062	1.00	48.28
ATOM	291	NZ	LYS	1510	0.318	-1.067	32.245	1.00	51.03
ATOM	292	C	LYS	1510	-0.813	-0.213	25.355	1.00	29.64
ATOM	293	O	LYS	1510	-0.521	-1.218	24.700	1.00	28.00
ATOM	294	N	VAL	1511	-0.904	1.004	24.836	1.00	30.10
ATOM	295	CA	VAL	1511	-0.625	1.305	23.446	1.00	30.13
ATOM	296	CB	VAL	1511	-1.951	1.464	22.636	1.00	31.39
ATOM	297	CG1	VAL	1511	-2.719	0.143	22.615	1.00	30.42
ATOM	298	CG2	VAL	1511	-2.829	2.629	23.223	1.00	28.08
ATOM	299	C	VAL	1511	0.150	2.626	23.365	1.00	30.51
ATOM	300	O	VAL	1511	0.274	3.346	24.360	1.00	31.09
ATOM	301	N	ALA	1512	0.679	2.935	22.185	1.00	28.30
ATOM	302	CA	ALA	1512	1.408	4.173	21.979	1.00	25.23
ATOM	303	CB	ALA	1512	2.740	3.889	21.331	1.00	23.82
ATOM	304	C	ALA	1512	0.535	5.012	21.057	1.00	25.50
ATOM	305	O	ALA	1512	0.033	4.515	20.061	1.00	27.06
ATOM	306	N	VAL	1513	0.351	6.281	21.404	1.00	29.37

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ATOM	307	CA	VAL	1513	-0.477	7.199	20.625	1.00	31.53
ATOM	308	CB	VAL	1513	-1.588	7.843	21.504	1.00	32.26
ATOM	309	CG1	VAL	1513	-2.453	8.775	20.684	1.00	34.37
ATOM	310	CG2	VAL	1513	-2.452	6.776	22.152	1.00	33.42
ATOM	311	C	VAL	1513	0.347	8.328	20.006	1.00	33.34
ATOM	312	O	VAL	1513	1.030	9.064	20.719	1.00	32.35
ATOM	313	N	LYS	1514	0.321	8.423	18.680	1.00	36.65
ATOM	314	CA	LYS	1514	1.022	9.466	17.929	1.00	37.26
ATOM	315	CB	LYS	1514	1.541	8.917	16.606	1.00	36.21
ATOM	316	CG	LYS	1514	2.524	7.792	16.800	1.00	39.32
ATOM	317	CD	LYS	1514	2.725	6.998	15.535	1.00	42.59
ATOM	318	CE	LYS	1514	3.245	7.860	14.416	1.00	44.71
ATOM	319	NZ	LYS	1514	4.408	8.680	14.844	1.00	38.78
ATOM	320	C	LYS	1514	0.020	10.574	17.653	1.00	37.21
ATOM	321	O	LYS	1514	-1.095	10.305	17.192	1.00	37.39
ATOM	322	N	MET	1515	0.433	11.812	17.908	1.00	39.05
ATOM	323	CA	MET	1515	-0.419	12.981	17.713	1.00	41.68
ATOM	324	CB	MET	1515	-1.162	13.299	18.991	1.00	41.07
ATOM	325	CG	MET	1515	-0.251	13.641	20.139	1.00	40.69
ATOM	326	SD	MET	1515	-1.271	13.763	21.571	1.00	41.18
ATOM	327	CE	MET	1515	-1.523	12.018	21.959	1.00	40.98
ATOM	328	C	MET	1515	0.397	14.197	17.321	1.00	44.66
ATOM	329	O	MET	1515	1.606	14.255	17.550	1.00	43.83
ATOM	330	N	LEU	1516	-0.288	15.182	16.747	1.00	50.63
ATOM	331	CA	LEU	1516	0.349	16.423	16.312	1.00	52.21
ATOM	332	CB	LEU	1516	-0.513	17.129	15.255	1.00	50.18
ATOM	333	CG	LEU	1516	-0.757	16.463	13.904	1.00	50.25
ATOM	334	CD1	LEU	1516	-1.733	17.298	13.114	1.00	51.02
ATOM	335	CD2	LEU	1516	0.555	16.329	13.163	1.00	51.60
ATOM	336	C	LEU	1516	0.549	17.391	17.473	1.00	54.25
ATOM	337	O	LEU	1516	-0.143	17.326	19.488	1.00	52.52
ATOM	338	N	LYS	1517	1.500	18.299	17.302	1.00	59.09
ATOM	339	CA	LYS	1517	1.773	19.315	18.313	1.00	62.57
ATOM	340	CB	LYS	1517	3.220	19.813	18.222	1.00	66.29
ATOM	341	CG	LYS	1517	4.281	18.810	18.663	1.00	70.96
ATOM	342	CD	LYS	1517	5.666	19.197	18.130	1.00	74.61
ATOM	343	CE	LYS	1517	6.711	18.118	18.414	1.00	78.21
ATOM	344	NZ	LYS	1517	8.020	18.410	17.751	1.00	77.95
ATOM	345	C	LYS	1517	0.824	20.474	18.037	1.00	63.07
ATOM	346	O	LYS	1517	0.226	20.557	16.960	1.00	63.68
ATOM	347	N	SER	1518	0.720	21.391	18.987	1.00	64.54
ATOM	348	CA	SER	1518	-0.167	22.543	18.848	1.00	67.29
ATOM	349	CB	SER	1518	-0.085	23.439	20.090	1.00	65.14
ATOM	350	C	SER	1518	0.124	23.382	17.609	1.00	69.48
ATOM	351	O	SER	1518	-0.798	23.843	16.938	1.00	71.85
ATOM	352	N	ASP	1519	1.402	23.530	17.280	1.00	70.88
ATOM	353	CA	ASP	1519	1.802	24.326	16.127	1.00	72.00
ATOM	354	CB	ASP	1519	3.162	24.973	16.385	1.00	72.61
ATOM	355	C	ASP	1519	1.861	23.548	14.817	1.00	72.32
ATOM	356	O	ASP	1519	2.432	24.035	13.844	1.00	73.72
ATOM	357	N	ALA	1520	1.322	22.332	14.798	1.00	72.11
ATOM	358	CA	ALA	1520	1.344	21.508	13.595	1.00	71.13

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ATOM	359	CB	ALA	1520	0.659	20.173	13.855	1.00	71.01
ATOM	360	C	ALA	1520	0.666	22.242	12.440	1.00	69.96
ATOM	361	O	ALA	1520	-0.314	22.962	12.639	1.00	71.41
ATOM	362	N	THR	1521	1.230	22.101	11.249	1.00	67.39
ATOM	363	CA	THR	1521	0.676	22.726	10.064	1.00	66.23
ATOM	364	CB	THR	1521	1.798	23.167	9.132	1.00	66.40
ATOM	365	OG1	THR	1521	2.521	22.016	8.680	1.00	70.07
ATOM	366	CG2	THR	1521	2.741	24.070	9.867	1.00	66.67
ATOM	367	C	THR	1521	-0.150	21.665	9.364	1.00	65.62
ATOM	368	O	THR	1521	-0.093	20.493	9.740	1.00	66.78
ATOM	369	N	GLU	1522	-0.893	22.057	8.330	1.00	63.60
ATOM	370	CA	GLU	1522	-1.698	21.095	7.584	1.00	62.25
ATOM	371	CB	GLU	1522	-2.560	21.802	6.531	1.00	64.02
ATOM	372	C	GLU	1522	-0.768	20.051	6.942	1.00	60.41
ATOM	373	O	GLU	1522	-1.161	18.906	6.738	1.00	61.94
ATOM	374	N	LYS	1523	0.475	20.441	6.662	1.00	56.47
ATOM	375	CA	LYS	1523	1.449	19.529	6.080	1.00	54.53
ATOM	376	CB	LYS	1523	2.739	20.273	5.713	1.00	57.44
ATOM	377	CG	LYS	1523	3.897	19.381	5.219	1.00	61.49
ATOM	378	CD	LYS	1523	3.482	18.451	4.071	1.00	64.66
ATOM	379	CE	LYS	1523	4.681	17.723	3.469	1.00	68.18
ATOM	380	NZ	LYS	1523	4.252	16.704	2.458	1.00	73.23
ATOM	381	C	LYS	1523	1.728	18.474	7.135	1.00	52.30
ATOM	382	O	LYS	1523	1.757	17.280	6.832	1.00	54.59
ATOM	383	N	ASP	1524	1.899	18.921	8.376	1.00	47.78
ATOM	384	CA	ASP	1524	2.147	18.023	9.493	1.00	45.55
ATOM	385	CB	ASP	1524	2.380	18.815	10.783	1.00	47.64
ATOM	386	CG	ASP	1524	3.744	19.511	10.817	1.00	49.50
ATOM	387	OD1	ASP	1524	3.849	20.580	11.460	1.00	47.22
ATOM	388	OD2	ASP	1524	4.715	18.984	10.230	1.00	52.84
ATOM	389	C	ASP	1524	0.968	17.054	9.661	1.00	43.55
ATOM	390	O	ASP	1524	1.157	15.890	10.007	1.00	43.98
ATOM	391	N	LEU	1525	-0.240	17.541	9.391	1.00	40.77
ATOM	392	CA	LEU	1525	-1.438	16.713	9.483	1.00	40.28
ATOM	393	CB	LEU	1525	-2.701	17.592	9.411	1.00	40.54
ATOM	394	CG	LEU	1525	-4.100	16.957	9.403	1.00	40.33
ATOM	395	CD1	LEU	1525	-4.289	15.933	10.514	1.00	42.75
ATOM	396	CD2	LEU	1525	-5.120	18.044	9.524	1.00	36.98
ATOM	397	C	LEU	1525	-1.417	15.699	8.343	1.00	40.19
ATOM	398	O	LEU	1525	-1.682	14.525	8.557	1.00	41.90
ATOM	399	N	SER	1526	-1.064	16.158	7.147	1.00	42.13
ATOM	400	CA	SER	1526	-1.002	15.315	5.954	1.00	44.75
ATOM	401	CB	SER	1526	-0.582	16.136	4.723	1.00	49.61
ATOM	402	OG	SER	1526	-1.538	17.100	4.352	1.00	59.95
ATOM	403	C	SER	1526	-0.007	14.193	6.144	1.00	42.71
ATOM	404	O	SER	1526	-0.297	13.047	5.840	1.00	45.33
ATOM	405	N	ASP	1527	1.167	14.527	6.655	1.00	40.97
ATOM	406	CA	ASP	1527	2.210	13.546	6.867	1.00	41.03
ATOM	407	CB	ASP	1527	3.497	14.235	7.316	1.00	45.30
ATOM	408	CG	ASP	1527	4.083	15.147	6.235	1.00	47.84
ATOM	409	OD1	ASP	1527	3.700	15.041	5.047	1.00	48.84
ATOM	410	OD2	ASP	1527	4.957	15.966	6.600	1.00	49.11

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ATOM	411	C	ASP	1527	1.782	12.485	7.858	1.00	39.01
ATOM	412	O	ASP	1527	2.021	11.298	7.651	1.00	40.04
ATOM	413	N	LEU	1528	1.094	12.917	8.909	1.00	35.93
ATOM	414	CA	LEU	1528	0.594	12.004	9.927	1.00	36.48
ATOM	415	CB	LEU	1528	-0.008	12.784	11.107	1.00	36.51
ATOM	416	CG	LEU	1528	-0.436	11.961	12.326	1.00	40.56
ATOM	417	CD1	LEU	1528	0.650	10.955	12.692	1.00	42.00
ATOM	418	CD2	LEU	1528	-0.770	12.877	13.499	1.00	38.25
ATOM	419	C	LEU	1528	-0.453	11.065	9.309	1.00	35.25
ATOM	420	O	LEU	1528	-0.442	9.855	9.566	1.00	36.37
ATOM	421	N	ILE	1529	-1.311	11.614	8.453	1.00	33.10
ATOM	422	CA	ILE	1529	-2.365	10.839	7.805	1.00	32.32
ATOM	423	CB	ILE	1529	-3.364	11.732	7.012	1.00	31.17
ATOM	424	CG2	ILE	1529	-4.311	10.861	6.187	1.00	32.01
ATOM	425	CG1	ILE	1529	-4.193	12.579	7.983	1.00	31.35
ATOM	426	CD1	ILE	1529	-5.024	13.662	7.335	1.00	32.59
ATOM	427	C	ILE	1529	-1.732	9.825	6.877	1.00	33.44
ATOM	428	O	ILE	1529	-2.148	8.667	6.860	1.00	35.41
ATOM	429	N	SER	1530	-0.733	10.269	6.108	1.00	33.40
ATOM	430	CA	SER	1530	0.007	9.414	5.171	1.00	34.34
ATOM	431	CB	SER	1530	1.126	10.197	4.495	1.00	38.37
ATOM	432	OG	SER	1530	0.605	11.332	3.835	1.00	46.02
ATOM	433	C	SER	1530	0.614	8.208	5.868	1.00	30.41
ATOM	434	O	SER	1530	0.494	7.083	5.376	1.00	30.50
ATOM	435	N	GLU	1531	1.256	8.449	7.010	1.00	27.40
ATOM	436	CA	GLU	1531	1.865	7.369	7.766	1.00	28.90
ATOM	437	CB	GLU	1531	2.629	7.907	8.973	1.00	28.45
ATOM	438	CG	GLU	1531	3.263	6.812	9.825	1.00	29.33
ATOM	439	CD	GLU	1531	4.094	7.344	10.979	1.00	31.14
ATOM	440	OE1	GLU	1531	4.913	6.561	11.495	1.00	33.14
ATOM	441	OE2	GLU	1531	3.940	8.522	11.378	1.00	31.11
ATOM	442	C	GLU	1531	0.824	6.351	8.215	1.00	30.88
ATOM	443	O	GLU	1531	1.118	5.146	8.259	1.00	32.35
ATOM	444	N	MET	1532	-0.377	6.832	8.553	1.00	29.86
ATOM	445	CA	MET	1532	-1.476	5.966	8.996	1.00	30.01
ATOM	446	CB	MET	1532	-2.608	6.800	9.596	1.00	29.58
ATOM	447	CG	MET	1532	-3.761	5.968	10.146	1.00	31.20
ATOM	448	SD	MET	1532	-5.095	6.973	10.779	1.00	29.37
ATOM	449	CE	MET	1532	-5.271	8.228	9.489	1.00	21.59
ATOM	450	C	MET	1532	-2.002	5.145	7.814	1.00	29.60
ATOM	451	O	MET	1532	-2.131	3.923	7.893	1.00	29.68
ATOM	452	N	GLU	1533	-2.257	5.824	6.702	1.00	30.38
ATOM	453	CA	GLU	1533	-2.755	5.176	5.495	1.00	30.12
ATOM	454	CB	GLU	1533	-2.987	6.221	4.423	1.00	25.79
ATOM	455	CG	GLU	1533	-4.117	7.154	4.784	1.00	26.67
ATOM	456	CD	GLU	1533	-5.420	6.405	5.064	1.00	29.90
ATOM	457	OE1	GLU	1533	-5.923	5.696	4.166	1.00	29.93
ATOM	458	OE2	GLU	1533	-5.939	6.518	6.197	1.00	29.10
ATOM	459	C	GLU	1533	-1.787	4.120	5.003	1.00	30.32
ATOM	460	O	GLU	1533	-2.197	3.043	4.563	1.00	32.06
ATOM	461	N	MET	1534	-0.500	4.435	5.136	1.00	29.97
ATOM	462	CA	MET	1534	0.606	3.571	4.737	1.00	31.22

ATOM	463	CB	MET	1534	1.918	4.305	4.985	1.00	33.86
ATOM	464	CG	MET	1534	3.118	3.487	4.675	1.00	40.40
ATOM	465	SD	MET	1534	3.528	3.627	2.982	1.00	48.27
ATOM	466	CE	MET	1534	5.215	4.257	3.155	1.00	42.49
ATOM	467	C	MET	1534	0.565	2.304	5.581	1.00	30.90
ATOM	468	O	MET	1534	0.596	1.193	5.050	1.00	33.24
ATOM	469	N	MET	1535	0.493	2.485	6.896	1.00	29.07
ATOM	470	CA	MET	1535	0.417	1.354	7.813	1.00	28.82
ATOM	471	CB	MET	1535	0.325	1.829	9.274	1.00	28.87
ATOM	472	CG	MET	1535	1.622	2.434	9.803	1.00	28.16
ATOM	473	SD	MET	1535	1.674	2.633	11.595	1.00	30.96
ATOM	474	CE	MET	1535	1.393	4.335	11.729	1.00	27.69
ATOM	475	C	MET	1535	-0.777	0.460	7.445	1.00	28.59
ATOM	476	O	MET	1535	-0.682	-0.774	7.530	1.00	30.37
ATOM	477	N	LYS	1536	-1.885	1.072	7.019	1.00	26.53
ATOM	478	CA	LYS	1536	-3.078	0.315	6.608	1.00	27.60
ATOM	479	CB	LYS	1536	-4.237	1.253	6.283	1.00	25.88
ATOM	480	CG	LYS	1536	-4.807	1.947	7.479	1.00	23.80
ATOM	481	CD	LYS	1536	-5.925	2.857	7.061	1.00	21.64
ATOM	482	CE	LYS	1536	-6.402	3.674	8.225	1.00	21.83
ATOM	483	NZ	LYS	1536	-7.469	4.594	7.796	1.00	26.27
ATOM	484	C	LYS	1536	-2.813	-0.573	5.397	1.00	27.49
ATOM	485	O	LYS	1536	-3.150	-1.756	5.393	1.00	29.24
ATOM	486	N	MET	1537	-2.186	-0.014	4.372	1.00	27.89
ATOM	487	CA	MET	1537	-1.890	-0.783	3.172	1.00	29.12
ATOM	488	CB	MET	1537	-1.321	0.136	2.085	1.00	32.72
ATOM	489	CG	MET	1537	-2.282	1.208	1.566	1.00	37.18
ATOM	490	SD	MET	1537	-3.740	0.505	0.744	1.00	43.17
ATOM	491	CE	MET	1537	-2.964	-0.152	-0.698	1.00	43.04
ATOM	492	C	MET	1537	-0.903	-1.920	3.447	1.00	29.58
ATOM	493	O	MET	1537	-1.102	-3.049	2.996	1.00	27.53
ATOM	494	N	ILE	1538	0.142	-1.626	4.223	1.00	28.64
ATOM	495	CA	ILE	1538	1.189	-2.609	4.533	1.00	26.88
ATOM	496	CB	ILE	1538	2.381	-1.948	5.280	1.00	25.23
ATOM	497	CG2	ILE	1538	3.380	-2.989	5.745	1.00	27.31
ATOM	498	CG1	ILE	1538	3.097	-0.968	4.345	1.00	22.70
ATOM	499	CD1	ILE	1538	4.445	-0.465	4.874	1.00	23.44
ATOM	500	C	ILE	1538	0.756	-3.911	5.224	1.00	26.75
ATOM	501	O	ILE	1538	1.274	-4.980	4.909	1.00	28.60
ATOM	502	N	GLY	1539	-0.200	-3.849	6.137	1.00	27.19
ATOM	503	CA	GLY	1539	-0.625	-5.069	6.812	1.00	26.88
ATOM	504	C	GLY	1539	0.207	-5.369	8.039	1.00	26.04
ATOM	505	O	GLY	1539	1.220	-4.708	8.281	1.00	27.96
ATOM	506	N	LYS	1540	-0.195	-6.396	8.788	1.00	23.25
ATOM	507	CA	LYS	1540	0.461	-6.781	10.052	1.00	21.53
ATOM	508	CB	LYS	1540	-0.573	-7.350	11.028	1.00	20.48
ATOM	509	CG	LYS	1540	-1.530	-6.346	11.563	1.00	28.42
ATOM	510	CD	LYS	1540	-2.542	-6.977	12.502	1.00	36.24
ATOM	511	CE	LYS	1540	-3.568	-5.942	12.994	1.00	41.05
ATOM	512	NZ	LYS	1540	-2.973	-4.847	13.836	1.00	41.25
ATOM	513	C	LYS	1540	1.577	-7.796	9.974	1.00	19.96
ATOM	514	O	LYS	1540	1.536	-8.723	9.176	1.00	21.51

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ATOM	515	N	HIS	1541	2.514	-7.670	10.905	1.00	19.82
ATOM	516	CA	HIS	1541	3.622	-8.613	11.040	1.00	21.35
ATOM	517	CB	HIS	1541	4.704	-8.411	9.972	1.00	21.39
ATOM	518	CG	HIS	1541	5.747	-9.490	9.963	1.00	17.07
ATOM	519	CD2	HIS	1541	5.810	-10.667	9.292	1.00	18.04
ATOM	520	ND1	HIS	1541	6.891	-9.428	10.727	1.00	19.05
ATOM	521	CE1	HIS	1541	7.609	-10.522	10.535	1.00	19.63
ATOM	522	NE2	HIS	1541	6.975	-11.293	9.668	1.00	18.32
ATOM	523	C	HIS	1541	4.198	-8.456	12.449	1.00	23.61
ATOM	524	O	HIS	1541	4.231	-7.352	13.002	1.00	25.66
ATOM	525	N	LYS	1542	4.587	-9.577	13.045	1.00	24.32
ATOM	526	CA	LYS	1542	5.141	-9.610	14.396	1.00	27.04
ATOM	527	CB	LYS	1542	5.578	-11.044	14.742	1.00	30.70
ATOM	528	CG	LYS	1542	6.130	-11.239	16.150	1.00	40.75
ATOM	529	CD	LYS	1542	6.380	-12.719	16.420	1.00	48.24
ATOM	530	CE	LYS	1542	6.995	-13.414	15.183	1.00	56.89
ATOM	531	NZ	LYS	1542	7.457	-14.831	15.421	1.00	60.99
ATOM	532	C	LYS	1542	6.318	-8.674	14.608	1.00	24.59
ATOM	533	O	LYS	1542	6.462	-8.067	15.676	1.00	23.35
ATOM	534	N	ASN	1543	7.147	-8.546	13.576	1.00	22.05
ATOM	535	CA	ASN	1543	8.333	-7.702	13.689	1.00	21.40
ATOM	536	CB	ASN	1543	9.558	-8.482	13.217	1.00	20.89
ATOM	537	CG	ASN	1543	9.721	-9.811	13.945	1.00	20.37
ATOM	538	OD1	ASN	1543	9.501	-10.883	13.372	1.00	24.97
ATOM	539	ND2	ASN	1543	10.016	-9.741	15.230	1.00	21.56
ATOM	540	C	ASN	1543	8.312	-6.268	13.155	1.00	20.38
ATOM	541	O	ASN	1543	9.353	-5.733	12.776	1.00	20.03
ATOM	542	N	ILE	1544	7.153	-5.624	13.180	1.00	20.02
ATOM	543	CA	ILE	1544	7.037	-4.226	12.771	1.00	21.14
ATOM	544	CB	ILE	1544	6.545	-4.029	11.292	1.00	22.97
ATOM	545	CG2	ILE	1544	7.436	-4.810	10.334	1.00	23.27
ATOM	546	CG1	ILE	1544	5.082	-4.447	11.096	1.00	22.85
ATOM	547	CD1	ILE	1544	4.485	-3.974	9.760	1.00	18.94
ATOM	548	C	ILE	1544	6.044	-3.590	13.757	1.00	20.02
ATOM	549	O	ILE	1544	5.342	-4.309	14.466	1.00	21.00
ATOM	550	N	ILE	1545	6.103	-2.275	13.943	1.00	20.09
ATOM	551	CA	ILE	1545	5.140	-1.608	14.826	1.00	22.82
ATOM	552	CB	ILE	1545	5.586	-0.161	15.198	1.00	23.07
ATOM	553	CG2	ILE	1545	4.399	0.652	15.718	1.00	21.94
ATOM	554	CG1	ILE	1545	6.759	-0.178	16.193	1.00	20.49
ATOM	555	CD1	ILE	1545	6.450	-0.730	17.579	1.00	15.00
ATOM	556	C	ILE	1545	3.853	-1.555	14.010	1.00	24.18
ATOM	557	O	ILE	1545	3.809	-0.954	12.920	1.00	25.68
ATOM	558	N	ASN	1546	2.829	-2.236	14.514	1.00	25.69
ATOM	559	CA	ASN	1546	1.528	-2.311	13.853	1.00	24.23
ATOM	560	CB	ASN	1546	0.866	-3.697	14.060	1.00	25.21
ATOM	561	CG	ASN	1546	1.690	-4.834	13.481	1.00	21.10
ATOM	562	OD1	ASN	1546	1.764	-4.997	12.274	1.00	23.44
ATOM	563	ND2	ASN	1546	2.324	-5.606	14.343	1.00	18.20
ATOM	564	C	ASN	1546	0.567	-1.235	14.325	1.00	23.12
ATOM	565	O	ASN	1546	0.709	-0.682	15.426	1.00	24.14
ATOM	566	N	LEU	1547	-0.382	-0.920	13.456	1.00	23.49

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ATOM	567	CA	LEU	1547	-1.417	0.069	13.718	1.00	24.50
ATOM	568	CB	LEU	1547	-1.976	0.597	12.378	1.00	21.63
ATOM	569	CG	LEU	1547	-3.189	1.535	12.353	1.00	22.37
ATOM	570	CD1	LEU	1547	-2.834	2.903	12.922	1.00	21.78
ATOM	571	CD2	LEU	1547	-3.714	1.660	10.930	1.00	21.31
ATOM	572	C	LEU	1547	-2.510	-0.681	14.495	1.00	26.70
ATOM	573	O	LEU	1547	-2.849	-1.823	14.160	1.00	28.96
ATOM	574	N	LEU	1548	-3.017	-0.082	15.565	1.00	25.96
ATOM	575	CA	LEU	1548	-4.047	-0.714	16.365	1.00	22.37
ATOM	576	CB	LEU	1548	-3.686	-0.682	17.868	1.00	17.76
ATOM	577	CG	LEU	1548	-2.346	-1.360	18.224	1.00	17.12
ATOM	578	CD1	LEU	1548	-2.150	-1.468	19.708	1.00	18.81
ATOM	579	CD2	LEU	1548	-2.266	-2.737	17.631	1.00	16.20
ATOM	580	C	LEU	1548	-5.395	-0.061	16.099	1.00	23.30
ATOM	581	O	LEU	1548	-6.418	-0.727	16.175	1.00	24.18
ATOM	582	N	GLY	1549	-5.395	1.228	15.758	1.00	21.53
ATOM	583	CA	GLY	1549	-6.636	1.933	15.485	1.00	22.47
ATOM	584	C	GLY	1549	-6.392	3.421	15.340	1.00	24.62
ATOM	585	O	GLY	1549	-5.245	3.835	15.163	1.00	25.06
ATOM	586	N	ALA	1550	-7.459	4.219	15.409	1.00	24.15
ATOM	587	CA	ALA	1550	-7.362	5.672	15.313	1.00	22.20
ATOM	588	CB	ALA	1550	-7.063	6.079	13.890	1.00	19.97
ATOM	589	C	ALA	1550	-8.602	6.415	15.802	1.00	23.75
ATOM	590	O	ALA	1550	-9.707	5.876	15.804	1.00	26.43
ATOM	591	N	CYS	1551	-8.383	7.660	16.213	1.00	25.34
ATOM	592	CA	CYS	1551	-9.425	8.590	16.678	1.00	27.17
ATOM	593	CB	CYS	1551	-9.160	9.045	18.127	1.00	26.84
ATOM	594	SG	CYS	1551	-9.246	7.802	19.448	1.00	30.32
ATOM	595	C	CYS	1551	-9.294	9.787	15.719	1.00	28.42
ATOM	596	O	CYS	1551	-8.364	10.575	15.827	1.00	27.28
ATOM	597	N	THR	1552	-10.145	9.823	14.702	1.00	30.47
ATOM	598	CA	THR	1552	-10.076	10.873	13.690	1.00	30.58
ATOM	599	CB	THR	1552	-10.061	10.219	12.280	1.00	30.58
ATOM	600	OG1	THR	1552	-11.266	9.465	12.096	1.00	31.11
ATOM	601	CG2	THR	1552	-8.895	9.255	12.151	1.00	27.59
ATOM	602	C	THR	1552	-11.241	11.847	13.695	1.00	32.24
ATOM	603	O	THR	1552	-11.192	12.911	13.070	1.00	28.56
ATOM	604	N	GLN	1553	-12.339	11.408	14.286	1.00	35.46
ATOM	605	CA	GLN	1553	-13.529	12.233	14.295	1.00	38.72
ATOM	606	CB	GLN	1553	-14.775	11.359	14.148	1.00	38.66
ATOM	607	CG	GLN	1553	-14.811	10.529	12.876	1.00	41.41
ATOM	608	CD	GLN	1553	-14.695	11.381	11.627	1.00	44.05
ATOM	609	OE1	GLN	1553	-15.442	12.345	11.445	1.00	45.08
ATOM	610	NE2	GLN	1553	-13.746	11.033	10.765	1.00	43.32
ATOM	611	C	GLN	1553	-13.658	13.168	15.483	1.00	41.20
ATOM	612	O	GLN	1553	-13.230	12.837	16.590	1.00	39.89
ATOM	613	N	ASP	1554	-14.225	14.344	15.219	1.00	44.03
ATOM	614	CA	ASP	1554	-14.474	15.356	16.237	1.00	46.94
ATOM	615	CB	ASP	1554	-15.778	15.028	16.976	1.00	49.94
ATOM	616	CG	ASP	1554	-17.007	15.262	16.122	1.00	56.68
ATOM	617	OD1	ASP	1554	-17.966	15.878	16.631	1.00	64.76
ATOM	618	OD2	ASP	1554	-17.030	14.829	14.947	1.00	60.79

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ATOM	619	C	ASP	1554	-13.343	15.563	17.244	1.00	47.24
ATOM	620	O	ASP	1554	-13.522	15.375	18.452	1.00	48.98
ATOM	621	N	GLY	1555	-12.182	15.966	16.747	1.00	44.00
ATOM	622	CA	GLY	1555	-11.062	16.185	17.638	1.00	41.07
ATOM	623	C	GLY	1555	-9.728	15.891	16.994	1.00	40.26
ATOM	624	O	GLY	1555	-9.663	15.567	15.810	1.00	39.72
ATOM	625	N	PRO	1556	-8.635	15.987	17.759	1.00	39.21
ATOM	626	CD	PRO	1556	-8.634	16.266	19.208	1.00	39.09
ATOM	627	CA	PRO	1556	-7.271	15.740	17.294	1.00	37.84
ATOM	628	CB	PRO	1556	-6.436	15.947	18.549	1.00	39.66
ATOM	629	CG	PRO	1556	-7.269	16.842	19.389	1.00	39.53
ATOM	630	C	PRO	1556	-7.094	14.314	16.806	1.00	37.75
ATOM	631	O	PRO	1556	-7.574	13.377	17.444	1.00	37.25
ATOM	632	N	LEU	1557	-6.379	14.153	15.699	1.00	36.09
ATOM	633	CA	LEU	1557	-6.112	12.844	15.124	1.00	34.69
ATOM	634	CB	LEU	1557	-5.458	13.010	13.741	1.00	32.25
ATOM	635	CG	LEU	1557	-4.962	11.774	12.972	1.00	31.23
ATOM	636	CD1	LEU	1557	-6.080	10.763	12.715	1.00	25.69
ATOM	637	CD2	LEU	1557	-4.339	12.219	11.669	1.00	28.21
ATOM	638	C	LEU	1557	-5.190	12.057	16.060	1.00	34.59
ATOM	639	O	LEU	1557	-4.173	12.578	16.524	1.00	32.09
ATOM	640	N	TYR	1558	-5.606	10.841	16.396	1.00	32.63
ATOM	641	CA	TYR	1558	-4.796	9.993	17.237	1.00	29.66
ATOM	642	CB	TYR	1558	-5.529	9.630	18.534	1.00	33.14
ATOM	643	CG	TYR	1558	-5.588	10.754	19.539	1.00	32.87
ATOM	644	CD1	TYR	1558	-6.583	10.793	20.517	1.00	34.58
ATOM	645	CE1	TYR	1558	-6.678	11.957	21.407	1.00	34.65
ATOM	646	CD2	TYR	1558	-4.678	11.805	19.483	1.00	35.69
ATOM	647	CE2	TYR	1558	-4.760	12.878	20.367	1.00	37.01
ATOM	648	CZ	TYR	1558	-5.766	12.899	21.324	1.00	37.52
ATOM	649	OH	TYR	1558	-5.868	13.986	22.164	1.00	40.19
ATOM	650	C	TYR	1558	-4.529	8.747	16.436	1.00	28.08
ATOM	651	O	TYR	1558	-5.467	8.137	15.924	1.00	30.12
ATOM	652	N	VAL	1559	-3.254	8.444	16.225	1.00	25.89
ATOM	653	CA	VAL	1559	-2.855	7.246	15.504	1.00	23.70
ATOM	654	CB	VAL	1559	-1.729	7.528	14.485	1.00	23.78
ATOM	655	CG1	VAL	1559	-1.456	6.282	13.623	1.00	20.75
ATOM	656	CG2	VAL	1559	-2.101	8.738	13.604	1.00	22.54
ATOM	657	C	VAL	1559	-2.358	6.311	16.596	1.00	23.47
ATOM	658	O	VAL	1559	-1.328	6.572	17.220	1.00	26.84
ATOM	659	N	ILE	1560	-3.146	5.283	16.889	1.00	23.58
ATOM	660	CA	ILE	1560	-2.818	4.316	17.928	1.00	23.75
ATOM	661	CB	ILE	1560	-4.112	3.732	18.552	1.00	22.67
ATOM	662	CG2	ILE	1560	-3.777	2.898	19.788	1.00	20.24
ATOM	663	CG1	ILE	1560	-5.063	4.884	18.904	1.00	20.09
ATOM	664	CD1	ILE	1560	-6.428	4.463	19.318	1.00	19.04
ATOM	665	C	ILE	1560	-1.954	3.181	17.356	1.00	27.39
ATOM	666	O	ILE	1560	-2.411	2.392	16.505	1.00	28.51
ATOM	667	N	VAL	1561	-0.720	3.089	17.840	1.00	26.76
ATOM	668	CA	VAL	1561	0.238	2.088	17.368	1.00	25.91
ATOM	669	CB	VAL	1561	1.445	2.801	16.653	1.00	24.50
ATOM	670	CG1	VAL	1561	0.952	3.480	15.397	1.00	13.55

ATOM	671	CG2	VAL	1561	2.054	3.870	17.551	1.00	20.39
ATOM	672	C	VAL	1561	0.693	1.151	18.519	1.00	24.80
ATOM	673	O	VAL	1561	0.397	1.417	19.696	1.00	25.26
ATOM	674	N	GLU	1562	1.349	0.032	18.192	1.00	22.30
ATOM	675	CA	GLU	1562	1.793	-0.901	19.230	1.00	21.49
ATOM	676	CB	GLU	1562	2.369	-2.179	18.630	1.00	16.65
ATOM	677	CG	GLU	1562	1.312	-3.115	18.092	1.00	19.71
ATOM	678	CD	GLU	1562	1.895	-4.356	17.460	1.00	21.58
ATOM	679	OE1	GLU	1562	1.281	-5.432	17.572	1.00	24.28
ATOM	680	OE2	GLU	1562	2.956	-4.260	16.825	1.00	23.74
ATOM	681	C	GLU	1562	2.802	-0.261	20.158	1.00	23.56
ATOM	682	O	GLU	1562	3.581	0.578	19.738	1.00	24.82
ATOM	683	N	TYR	1563	2.787	-0.665	21.422	1.00	26.96
ATOM	684	CA	TYR	1563	3.677	-0.132	22.442	1.00	28.98
ATOM	685	CB	TYR	1563	2.907	0.035	23.744	1.00	30.34
ATOM	686	CG	TYR	1563	3.744	0.456	24.929	1.00	33.86
ATOM	687	CD1	TYR	1563	4.457	1.653	24.915	1.00	36.58
ATOM	688	CE1	TYR	1563	5.195	2.069	26.021	1.00	36.89
ATOM	689	CD2	TYR	1563	3.787	-0.322	26.082	1.00	34.25
ATOM	690	CE2	TYR	1563	4.522	0.080	27.186	1.00	34.47
ATOM	691	CZ	TYR	1563	5.219	1.273	27.150	1.00	37.08
ATOM	692	OH	TYR	1563	5.965	1.662	28.228	1.00	44.10
ATOM	693	C	TYR	1563	4.884	-1.043	22.668	1.00	30.53
ATOM	694	O	TYR	1563	4.745	-2.269	22.751	1.00	30.66
ATOM	695	N	ALA	1564	6.068	-0.440	22.779	1.00	31.09
ATOM	696	CA	ALA	1564	7.303	-1.192	22.998	1.00	31.00
ATOM	697	CB	ALA	1564	8.236	-1.026	21.792	1.00	30.82
ATOM	698	C	ALA	1564	7.940	-0.663	24.283	1.00	29.32
ATOM	699	O	ALA	1564	8.703	0.309	24.274	1.00	32.26
ATOM	700	N	SER	1565	7.603	-1.303	25.389	1.00	29.55
ATOM	701	CA	SER	1565	8.059	-0.884	26.712	1.00	30.89
ATOM	702	CB	SER	1565	7.392	-1.729	27.792	1.00	29.79
ATOM	703	OG	SER	1565	7.704	-3.094	27.611	1.00	30.94
ATOM	704	C	SER	1565	9.547	-0.840	26.986	1.00	31.39
ATOM	705	O	SER	1565	9.978	-0.150	27.902	1.00	35.74
ATOM	706	N	LYS	1566	10.340	-1.576	26.229	1.00	30.03
ATOM	707	CA	LYS	1566	11.756	-1.560	26.495	1.00	28.80
ATOM	708	CB	LYS	1566	12.322	-2.973	26.447	1.00	28.98
ATOM	709	CG	LYS	1566	11.756	-3.842	27.563	1.00	25.35
ATOM	710	CD	LYS	1566	12.208	-5.279	27.459	1.00	30.93
ATOM	711	CE	LYS	1566	11.875	-6.001	28.747	1.00	31.41
ATOM	712	NZ	LYS	1566	12.315	-7.421	28.716	1.00	32.83
ATOM	713	C	LYS	1566	12.529	-0.595	25.623	1.00	29.93
ATOM	714	O	LYS	1566	13.756	-0.672	25.544	1.00	30.89
ATOM	715	N	GLY	1567	11.799	0.322	24.979	1.00	30.67
ATOM	716	CA	GLY	1567	12.423	1.328	24.138	1.00	28.44
ATOM	717	C	GLY	1567	13.136	0.874	22.875	1.00	27.19
ATOM	718	O	GLY	1567	12.919	-0.235	22.395	1.00	25.36
ATOM	719	N	ASN	1568	14.011	1.731	22.352	1.00	28.39
ATOM	720	CA	ASN	1568	14.735	1.421	21.130	1.00	28.41
ATOM	721	CB	ASN	1568	15.188	2.698	20.418	1.00	30.32
ATOM	722	CG	ASN	1568	16.396	3.352	21.058	1.00	33.42

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ATOM	723	OD1	ASN	1568	17.418	2.720	21.317	1.00	35.16
ATOM	724	ND2	ASN	1568	16.328	4.661	21.203	1.00	36.23
ATOM	725	C	ASN	1568	15.884	0.443	21.314	1.00	28.34
ATOM	726	O	ASN	1568	16.478	0.373	22.388	1.00	30.67
ATOM	727	N	LEU	1569	16.212	-0.270	20.244	1.00	27.65
ATOM	728	CA	LEU	1569	17.269	-1.270	20.247	1.00	29.10
ATOM	729	CB	LEU	1569	17.311	-1.974	18.880	1.00	27.49
ATOM	730	CG	LEU	1569	18.292	-3.130	18.657	1.00	28.82
ATOM	731	CD1	LEU	1569	18.236	-4.140	19.825	1.00	24.68
ATOM	732	CD2	LEU	1569	17.994	-3.791	17.316	1.00	22.26
ATOM	733	C	LEU	1569	18.667	-0.790	20.676	1.00	29.37
ATOM	734	O	LEU	1569	19.389	-1.525	21.355	1.00	29.72
ATOM	735	N	ARG	1570	19.058	0.425	20.303	1.00	30.89
ATOM	736	CA	ARG	1570	20.374	0.943	20.689	1.00	33.01
ATOM	737	CB	ARG	1570	20.591	2.353	20.121	1.00	30.95
ATOM	738	CG	ARG	1570	21.896	2.983	20.584	1.00	38.85
ATOM	739	CD	ARG	1570	21.968	4.472	20.303	1.00	43.03
ATOM	740	NE	ARG	1570	20.749	5.192	20.670	1.00	53.34
ATOM	741	CZ	ARG	1570	20.404	5.573	21.905	1.00	57.49
ATOM	742	NH1	ARG	1570	21.184	5.310	22.955	1.00	55.59
ATOM	743	NH2	ARG	1570	19.272	6.252	22.086	1.00	59.53
ATOM	744	C	ARG	1570	20.475	0.947	22.229	1.00	33.82
ATOM	745	O	ARG	1570	21.351	0.296	22.817	1.00	33.93
ATOM	746	N	GLU	1571	19.528	1.639	22.865	1.00	33.91
ATOM	747	CA	GLU	1571	19.435	1.746	24.317	1.00	32.59
ATOM	748	CB	GLU	1571	18.177	2.524	24.676	1.00	36.40
ATOM	749	CG	GLU	1571	18.174	3.958	24.175	1.00	45.91
ATOM	750	CD	GLU	1571	16.822	4.654	24.328	1.00	52.95
ATOM	751	OE1	GLU	1571	15.793	3.959	24.529	1.00	54.50
ATOM	752	OE2	GLU	1571	16.792	5.905	24.222	1.00	55.17
ATOM	753	C	GLU	1571	19.380	0.361	24.959	1.00	31.40
ATOM	754	O	GLU	1571	20.115	0.054	25.895	1.00	31.09
ATOM	755	N	TYR	1572	18.503	-0.477	24.433	1.00	29.24
ATOM	756	CA	TYR	1572	18.334	-1.835	24.920	1.00	27.43
ATOM	757	CB	TYR	1572	17.387	-2.590	23.991	1.00	26.41
ATOM	758	CG	TYR	1572	17.196	-4.045	24.311	1.00	23.13
ATOM	759	CD1	TYR	1572	16.224	-4.448	25.216	1.00	28.16
ATOM	760	CE1	TYR	1572	15.983	-5.784	25.456	1.00	28.32
ATOM	761	CD2	TYR	1572	17.936	-5.024	23.665	1.00	20.00
ATOM	762	CE2	TYR	1572	17.699	-6.361	23.899	1.00	22.28
ATOM	763	CZ	TYR	1572	16.721	-6.731	24.801	1.00	26.53
ATOM	764	OH	TYR	1572	16.479	-8.058	25.055	1.00	30.25
ATOM	765	C	TYR	1572	19.671	-2.564	24.960	1.00	30.90
ATOM	766	O	TYR	1572	19.953	-3.323	25.901	1.00	30.68
ATOM	767	N	LEU	1573	20.487	-2.337	23.933	1.00	31.27
ATOM	768	CA	LEU	1573	21.776	-2.995	23.841	1.00	33.33
ATOM	769	CB	LEU	1573	22.287	-2.975	22.399	1.00	30.85
ATOM	770	CG	LEU	1573	21.643	-3.908	21.370	1.00	26.92
ATOM	771	CD1	LEU	1573	22.144	-3.546	19.980	1.00	22.76
ATOM	772	CD2	LEU	1573	21.939	-5.372	21.695	1.00	25.82
ATOM	773	C	LEU	1573	22.801	-2.390	24.791	1.00	36.07
ATOM	774	O	LEU	1573	23.544	-3.117	25.457	1.00	36.40

ATOM	775	N	GLN	1574	22.815	-1.065	24.887	1.00	37.25
ATOM	776	CA	GLN	1574	23.763	-0.391	25.759	1.00	37.41
ATOM	777	CB	GLN	1574	23.722	1.119	25.522	1.00	38.07
ATOM	778	CG	GLN	1574	24.240	1.529	24.147	1.00	40.76
ATOM	779	CD	GLN	1574	24.046	3.009	23.851	1.00	44.73
ATOM	780	OE1	GLN	1574	23.391	3.740	24.597	1.00	46.47
ATOM	781	NE2	GLN	1574	24.606	3.452	22.732	1.00	46.93
ATOM	782	C	GLN	1574	23.502	-0.711	27.233	1.00	37.80
ATOM	783	O	GLN	1574	24.431	-0.988	27.990	1.00	38.55
ATOM	784	N	ALA	1575	22.229	-0.742	27.617	1.00	37.28
ATOM	785	CA	ALA	1575	21.846	-1.021	28.987	1.00	35.47
ATOM	786	CB	ALA	1575	20.394	-0.669	29.178	1.00	31.42
ATOM	787	C	ALA	1575	22.102	-2.473	29.424	1.00	38.30
ATOM	788	O	ALA	1575	21.758	-2.843	30.544	1.00	41.11
ATOM	789	N	ARG	1576	22.647	-3.299	28.528	1.00	37.59
ATOM	790	CA	ARG	1576	22.943	-4.687	28.869	1.00	37.23
ATOM	791	CB	ARG	1576	22.027	-5.636	28.111	1.00	36.82
ATOM	792	CG	ARG	1576	20.599	-5.481	28.561	1.00	34.61
ATOM	793	CD	ARG	1576	19.649	-6.146	27.640	1.00	31.82
ATOM	794	NE	ARG	1576	18.308	-6.147	28.201	1.00	31.54
ATOM	795	CZ	ARG	1576	17.590	-5.051	28.426	1.00	33.71
ATOM	796	NH1	ARG	1576	18.086	-3.855	28.149	1.00	33.68
ATOM	797	NH2	ARG	1576	16.337	-5.160	28.857	1.00	38.97
ATOM	798	C	ARG	1576	24.405	-5.052	28.683	1.00	38.53
ATOM	799	O	ARG	1576	24.790	-6.231	28.700	1.00	38.39
ATOM	800	N	ARG	1577	25.226	-4.017	28.538	1.00	39.28
ATOM	801	CA	ARG	1577	26.661	-4.185	28.394	1.00	39.33
ATOM	802	CB	ARG	1577	27.306	-2.855	27.998	1.00	35.44
ATOM	803	CG	ARG	1577	27.048	-2.402	26.584	1.00	33.45
ATOM	804	CD	ARG	1577	27.696	-1.042	26.330	1.00	32.83
ATOM	805	NE	ARG	1577	27.798	-0.747	24.897	1.00	36.69
ATOM	806	CZ	ARG	1577	28.284	0.385	24.384	1.00	36.99
ATOM	807	NH1	ARG	1577	28.719	1.359	25.175	1.00	40.35
ATOM	808	NH2	ARG	1577	28.346	0.539	23.065	1.00	36.53
ATOM	809	C	ARG	1577	27.222	-4.594	29.754	1.00	41.24
ATOM	810	O	ARG	1577	26.652	-4.244	30.796	1.00	41.03
ATOM	811	N	PRO	1578	28.307	-5.381	29.769	1.00	44.39
ATOM	812	CD	PRO	1578	29.038	-6.041	28.667	1.00	44.50
ATOM	813	CA	PRO	1578	28.877	-5.766	31.066	1.00	44.89
ATOM	814	CB	PRO	1578	29.933	-6.809	30.686	1.00	42.49
ATOM	815	CG	PRO	1578	30.352	-6.391	29.327	1.00	43.63
ATOM	816	C	PRO	1578	29.490	-4.493	31.672	1.00	45.20
ATOM	817	O	PRO	1578	29.814	-3.538	30.947	1.00	44.68
ATOM	818	N	PRO	1579	29.604	-4.432	33.003	1.00	46.51
ATOM	819	CD	PRO	1579	29.208	-5.463	33.981	1.00	46.36
ATOM	820	CA	PRO	1579	30.169	-3.265	33.685	1.00	47.56
ATOM	821	CB	PRO	1579	30.175	-3.708	35.141	1.00	46.45
ATOM	822	CG	PRO	1579	28.997	-4.638	35.205	1.00	47.51
ATOM	823	C	PRO	1579	31.575	-2.904	33.200	1.00	50.19
ATOM	824	O	PRO	1579	32.481	-3.739	33.196	1.00	53.53
ATOM	825	N	ALA	1592	19.097	-5.342	32.478	1.00	60.30
ATOM	826	CA	ALA	1592	20.535	-5.076	32.445	1.00	59.47

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ATOM	827	CB	ALA	1592	20.975	-4.338	33.715	1.00	61.58
ATOM	828	C	ALA	1592	21.367	-6.350	32.252	1.00	58.15
ATOM	829	O	ALA	1592	22.543	-6.285	31.879	1.00	59.09
ATOM	830	N	ALA	1593	20.754	-7.510	32.479	1.00	55.79
ATOM	831	CA	ALA	1593	21.457	-8.775	32.324	1.00	55.06
ATOM	832	CB	ALA	1593	20.519	-9.939	32.604	1.00	57.05
ATOM	833	C	ALA	1593	22.053	-8.897	30.924	1.00	53.57
ATOM	834	O	ALA	1593	21.402	-8.598	29.926	1.00	53.85
ATOM	835	N	GLN	1594	23.303	-9.336	30.862	1.00	53.22
ATOM	836	CA	GLN	1594	24.004	-9.490	29.599	1.00	50.13
ATOM	837	CB	GLN	1594	25.400	-10.082	29.832	1.00	50.73
ATOM	838	CG	GLN	1594	26.308	-9.253	30.743	1.00	54.69
ATOM	839	CD	GLN	1594	27.550	-10.019	31.217	1.00	57.79
ATOM	840	OE1	GLN	1594	28.075	-10.900	30.524	1.00	58.82
ATOM	841	NE2	GLN	1594	28.026	-9.673	32.407	1.00	59.53
ATOM	842	C	GLN	1594	23.210	-10.374	28.637	1.00	47.73
ATOM	843	O	GLN	1594	22.427	-11.241	29.054	1.00	47.09
ATOM	844	N	LEU	1595	23.418	-10.133	27.350	1.00	45.64
ATOM	845	CA	LEU	1595	22.758	-10.880	26.292	1.00	42.00
ATOM	846	CB	LEU	1595	22.405	-9.947	25.122	1.00	37.98
ATOM	847	CG	LEU	1595	21.345	-8.894	25.446	1.00	37.70
ATOM	848	CD1	LEU	1595	21.568	-7.611	24.660	1.00	33.34
ATOM	849	CD2	LEU	1595	19.971	-9.479	25.222	1.00	32.84
ATOM	850	C	LEU	1595	23.729	-11.944	25.828	1.00	40.92
ATOM	851	O	LEU	1595	24.944	-11.745	25.855	1.00	41.12
ATOM	852	N	SER	1596	23.201	-13.103	25.471	1.00	40.09
ATOM	853	CA	SER	1596	24.044	-14.178	24.985	1.00	38.93
ATOM	854	CB	SER	1596	23.388	-15.535	25.235	1.00	37.45
ATOM	855	OG	SER	1596	22.158	-15.662	24.545	1.00	39.49
ATOM	856	C	SER	1596	24.302	-13.987	23.499	1.00	39.41
ATOM	857	O	SER	1596	23.634	-13.183	22.832	1.00	39.51
ATOM	858	N	SER	1597	25.266	-14.738	22.977	1.00	39.17
ATOM	859	CA	SER	1597	25.587	-14.667	21.563	1.00	40.23
ATOM	860	CB	SER	1597	26.740	-15.611	21.230	1.00	39.96
ATOM	861	OG	SER	1597	27.865	-15.339	22.048	1.00	46.60
ATOM	862	C	SER	1597	24.347	-15.057	20.773	1.00	39.65
ATOM	863	O	SER	1597	24.066	-14.469	19.725	1.00	41.13
ATOM	864	N	LYS	1598	23.590	-16.023	21.291	1.00	36.82
ATOM	865	CA	LYS	1598	22.390	-16.467	20.611	1.00	36.17
ATOM	866	CB	LYS	1598	21.827	-17.742	21.217	1.00	36.19
ATOM	867	CG	LYS	1598	21.030	-18.562	20.180	1.00	39.59
ATOM	868	CD	LYS	1598	20.150	-19.623	20.830	1.00	37.49
ATOM	869	CE	LYS	1598	19.769	-20.719	19.855	1.00	39.64
ATOM	870	NZ	LYS	1598	20.976	-21.437	19.380	1.00	41.43
ATOM	871	C	LYS	1598	21.340	-15.381	20.649	1.00	37.72
ATOM	872	O	LYS	1598	20.604	-15.213	19.677	1.00	39.82
ATOM	873	N	ASP	1599	21.291	-14.627	21.752	1.00	36.20
ATOM	874	CA	ASP	1599	20.331	-13.530	21.907	1.00	33.96
ATOM	875	CB	ASP	1599	20.456	-12.884	23.279	1.00	35.66
ATOM	876	CG	ASP	1599	19.913	-13.744	24.394	1.00	36.18
ATOM	877	OD1	ASP	1599	20.365	-13.565	25.544	1.00	39.14
ATOM	878	OD2	ASP	1599	19.036	-14.593	24.128	1.00	33.40

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ATOM	879	C	ASP	1599	20.595	-12.471	20.857	1.00	33.57
ATOM	880	O	ASP	1599	19.660	-11.953	20.225	1.00	32.60
ATOM	881	N	LEU	1600	21.871	-12.123	20.706	1.00	32.82
ATOM	882	CA	LEU	1600	22.304	-11.121	19.735	1.00	31.14
ATOM	883	CB	LEU	1600	23.804	-10.850	19.916	1.00	30.23
ATOM	884	CG	LEU	1600	24.174	-10.153	21.242	1.00	27.52
ATOM	885	CD1	LEU	1600	25.660	-9.877	21.324	1.00	24.11
ATOM	886	CD2	LEU	1600	23.408	-8.857	21.369	1.00	21.94
ATOM	887	C	LEU	1600	21.964	-11.523	18.291	1.00	29.24
ATOM	888	O	LEU	1600	21.385	-10.734	17.541	1.00	27.61
ATOM	889	N	VAL	1601	22.271	-12.764	17.930	1.00	27.38
ATOM	890	CA	VAL	1601	21.983	-13.268	16.597	1.00	27.26
ATOM	891	CB	VAL	1601	22.648	-14.649	16.345	1.00	30.47
ATOM	892	CG1	VAL	1601	22.403	-15.104	14.921	1.00	28.72
ATOM	893	CG2	VAL	1601	24.156	-14.568	16.593	1.00	29.92
ATOM	894	C	VAL	1601	20.474	-13.353	16.399	1.00	26.23
ATOM	895	O	VAL	1601	19.991	-13.147	15.295	1.00	25.54
ATOM	896	N	SER	1602	19.733	-13.590	17.478	1.00	27.43
ATOM	897	CA	SER	1602	18.277	-13.671	17.406	1.00	27.09
ATOM	898	CB	SER	1602	17.731	-14.259	18.694	1.00	29.02
ATOM	899	OG	SER	1602	16.317	-14.306	18.646	1.00	35.77
ATOM	900	C	SER	1602	17.669	-12.280	17.149	1.00	26.87
ATOM	901	O	SER	1602	16.643	-12.141	16.465	1.00	25.13
ATOM	902	N	CYS	1603	18.289	-11.262	17.737	1.00	26.09
ATOM	903	CA	CYS	1603	17.878	-9.871	17.561	1.00	24.81
ATOM	904	CB	CYS	1603	18.797	-8.937	18.350	1.00	23.87
ATOM	905	SG	CYS	1603	18.512	-7.186	18.059	0.50	24.17
ATOM	906	C	CYS	1603	17.994	-9.517	16.090	1.00	25.24
ATOM	907	O	CYS	1603	17.083	-8.932	15.520	1.00	27.48
ATOM	908	N	ALA	1604	19.138	-9.854	15.492	1.00	26.80
ATOM	909	CA	ALA	1604	19.422	-9.592	14.073	1.00	26.15
ATOM	910	CB	ALA	1604	20.851	-10.035	13.741	1.00	24.35
ATOM	911	C	ALA	1604	18.419	-10.302	13.168	1.00	26.61
ATOM	912	O	ALA	1604	17.894	-9.713	12.226	1.00	28.81
ATOM	913	N	TYR	1605	18.130	-11.557	13.488	1.00	27.10
ATOM	914	CA	TYR	1605	17.175	-12.359	12.730	1.00	27.02
ATOM	915	CB	TYR	1605	17.104	-13.751	13.334	1.00	27.35
ATOM	916	CG	TYR	1605	15.997	-14.608	12.789	1.00	31.67
ATOM	917	CD1	TYR	1605	16.109	-15.244	11.546	1.00	32.96
ATOM	918	CE1	TYR	1605	15.069	-16.049	11.053	1.00	29.27
ATOM	919	CD2	TYR	1605	14.830	-14.797	13.520	1.00	31.42
ATOM	920	CE2	TYR	1605	13.801	-15.596	13.038	1.00	28.20
ATOM	921	CZ	TYR	1605	13.922	-16.212	11.810	1.00	29.20
ATOM	922	OH	TYR	1605	12.855	-16.944	11.364	1.00	27.90
ATOM	923	C	TYR	1605	15.766	-11.735	12.658	1.00	27.90
ATOM	924	O	TYR	1605	15.180	-11.635	11.578	1.00	28.40
ATOM	925	N	GLN	1606	15.231	-11.319	13.807	1.00	27.12
ATOM	926	CA	GLN	1606	13.907	-10.699	13.892	1.00	25.32
ATOM	927	CB	GLN	1606	13.561	-10.383	15.342	1.00	24.31
ATOM	928	CG	GLN	1606	13.329	-11.608	16.210	1.00	25.05
ATOM	929	CD	GLN	1606	13.052	-11.243	17.649	1.00	26.35
ATOM	930	OE1	GLN	1606	12.087	-10.542	17.944	1.00	26.11

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ATOM	931	NE2	GLN	1606	13.917	-11.684	18.551	1.00	27.77
ATOM	932	C	GLN	1606	13.849	-9.415	13.078	1.00	27.52
ATOM	933	O	GLN	1606	12.825	-9.089	12.455	1.00	27.87
ATOM	934	N	VAL	1607	14.943	-8.662	13.122	1.00	27.90
ATOM	935	CA	VAL	1607	15.053	-7.419	12.359	1.00	26.41
ATOM	936	CB	VAL	1607	16.337	-6.661	12.731	1.00	25.61
ATOM	937	CG1	VAL	1607	16.545	-5.457	11.800	1.00	27.37
ATOM	938	CG2	VAL	1607	16.277	-6.224	14.190	1.00	21.50
ATOM	939	C	VAL	1607	15.035	-7.718	10.860	1.00	26.09
ATOM	940	O	VAL	1607	14.337	-7.046	10.096	1.00	28.48
ATOM	941	N	ALA	1608	15.795	-8.722	10.435	1.00	23.05
ATOM	942	CA	ALA	1608	15.812	-9.079	9.027	1.00	20.32
ATOM	943	CB	ALA	1608	16.823	-10.145	8.783	1.00	14.95
ATOM	944	C	ALA	1608	14.418	-9.558	8.600	1.00	23.08
ATOM	945	O	ALA	1608	14.033	-9.405	7.432	1.00	23.91
ATOM	946	N	ARG	1609	13.671	-10.169	9.530	1.00	24.57
ATOM	947	CA	ARG	1609	12.314	-10.628	9.246	1.00	24.30
ATOM	948	CB	ARG	1609	11.822	-11.577	10.326	1.00	26.13
ATOM	949	CG	ARG	1609	12.278	-12.979	10.114	1.00	31.07
ATOM	950	CD	ARG	1609	11.449	-13.885	10.939	1.00	36.13
ATOM	951	NE	ARG	1609	10.771	-14.865	10.115	1.00	38.37
ATOM	952	CZ	ARG	1609	9.931	-15.778	10.594	1.00	37.95
ATOM	953	NH1	ARG	1609	9.674	-15.828	11.898	1.00	35.31
ATOM	954	NH2	ARG	1609	9.353	-16.649	9.776	1.00	37.85
ATOM	955	C	ARG	1609	11.318	-9.490	9.065	1.00	22.34
ATOM	956	O	ARG	1609	10.470	-9.542	8.160	1.00	24.57
ATOM	957	N	GLY	1610	11.375	-8.500	9.948	1.00	20.52
ATOM	958	CA	GLY	1610	10.497	-7.353	9.827	1.00	19.33
ATOM	959	C	GLY	1610	10.732	-6.715	8.464	1.00	20.04
ATOM	960	O	GLY	1610	9.794	-6.455	7.693	1.00	19.10
ATOM	961	N	MET	1611	12.011	-6.545	8.130	1.00	18.21
ATOM	962	CA	MET	1611	12.423	-5.970	6.851	1.00	20.32
ATOM	963	CB	MET	1611	13.925	-5.737	6.838	1.00	19.20
ATOM	964	CG	MET	1611	14.371	-4.547	7.694	1.00	20.83
ATOM	965	SD	MET	1611	13.449	-2.960	7.422	1.00	25.39
ATOM	966	CE	MET	1611	13.869	-2.525	5.757	1.00	18.67
ATOM	967	C	MET	1611	12.024	-6.843	5.670	1.00	23.98
ATOM	968	O	MET	1611	11.608	-6.332	4.613	1.00	24.13
ATOM	969	N	GLU	1612	12.141	-8.162	5.825	1.00	25.76
ATOM	970	CA	GLU	1612	11.759	-9.059	4.743	1.00	25.49
ATOM	971	CB	GLU	1612	11.980	-10.522	5.110	1.00	26.09
ATOM	972	CG	GLU	1612	11.587	-11.468	3.968	1.00	26.56
ATOM	973	CD	GLU	1612	11.735	-12.942	4.313	1.00	29.26
ATOM	974	OE1	GLU	1612	11.386	-13.316	5.448	1.00	29.10
ATOM	975	OE2	GLU	1612	12.190	-13.725	3.443	1.00	31.11
ATOM	976	C	GLU	1612	10.283	-8.821	4.398	1.00	26.29
ATOM	977	O	GLU	1612	9.916	-8.728	3.226	1.00	28.46
ATOM	978	N	TYR	1613	9.437	-8.700	5.422	1.00	24.78
ATOM	979	CA	TYR	1613	8.003	-8.456	5.212	1.00	23.07
ATOM	980	CB	TYR	1613	7.263	-8.526	6.549	1.00	23.75
ATOM	981	CG	TYR	1613	5.785	-8.218	6.449	1.00	20.80
ATOM	982	CD1	TYR	1613	4.880	-9.213	6.062	1.00	20.97

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ATOM	983	CE1	TYR	1613	3.517	-8.944	5.958	1.00	20.03
ATOM	984	CD2	TYR	1613	5.289	-6.938	6.731	1.00	19.72
ATOM	985	CE2	TYR	1613	3.926	-6.661	6.628	1.00	21.87
ATOM	986	CZ	TYR	1613	3.046	-7.672	6.244	1.00	24.87
ATOM	987	OH	TYR	1613	1.694	-7.420	6.161	1.00	24.37
ATOM	988	C	TYR	1613	7.766	-7.094	4.550	1.00	21.68
ATOM	989	O	TYR	1613	6.970	-6.979	3.615	1.00	20.20
ATOM	990	N	LEU	1614	8.436	-6.065	5.062	1.00	21.72
ATOM	991	CA	LEU	1614	8.321	-4.713	4.519	1.00	20.42
ATOM	992	CB	LEU	1614	9.169	-3.747	5.350	1.00	17.68
ATOM	993	CG	LEU	1614	8.607	-3.395	6.733	1.00	18.47
ATOM	994	CD1	LEU	1614	9.504	-2.425	7.470	1.00	16.59
ATOM	995	CD2	LEU	1614	7.230	-2.795	6.558	1.00	14.07
ATOM	996	C	LEU	1614	8.729	-4.676	3.043	1.00	21.70
ATOM	997	O	LEU	1614	8.073	-4.038	2.211	1.00	22.25
ATOM	998	N	ALA	1615	9.819	-5.366	2.729	1.00	21.55
ATOM	999	CA	ALA	1615	10.313	-5.435	1.355	1.00	20.52
ATOM	1000	CB	ALA	1615	11.625	-6.207	1.292	1.00	19.78
ATOM	1001	C	ALA	1615	9.264	-6.098	0.491	1.00	19.98
ATOM	1002	O	ALA	1615	8.945	-5.587	-0.579	1.00	20.14
ATOM	1003	N	SER	1616	8.692	-7.205	0.972	1.00	20.65
ATOM	1004	CA	SER	1616	7.660	-7.919	0.207	1.00	19.59
ATOM	1005	CB	SER	1616	7.283	-9.217	0.912	1.00	15.96
ATOM	1006	OG	SER	1616	6.415	-8.966	2.007	1.00	16.62
ATOM	1007	C	SER	1616	6.397	-7.062	-0.018	1.00	22.05
ATOM	1008	O	SER	1616	5.650	-7.266	-0.975	1.00	23.62
ATOM	1009	N	LYS	1617	6.136	-6.135	0.895	1.00	23.39
ATOM	1010	CA	LYS	1617	4.997	-5.237	0.779	1.00	23.02
ATOM	1011	CB	LYS	1617	4.436	-4.881	2.160	1.00	21.50
ATOM	1012	CG	LYS	1617	3.709	-6.046	2.851	1.00	24.94
ATOM	1013	CD	LYS	1617	2.463	-6.448	2.059	1.00	26.57
ATOM	1014	CE	LYS	1617	1.691	-7.571	2.725	1.00	31.05
ATOM	1015	NZ	LYS	1617	2.401	-8.852	2.601	1.00	38.73
ATOM	1016	C	LYS	1617	5.346	-3.981	-0.017	1.00	24.01
ATOM	1017	O	LYS	1617	4.588	-3.007	-0.013	1.00	28.15
ATOM	1018	N	LYS	1618	6.496	-4.002	-0.679	1.00	23.84
ATOM	1019	CA	LYS	1618	6.957	-2.883	-1.528	1.00	24.05
ATOM	1020	CB	LYS	1618	5.871	-2.513	-2.555	1.00	25.74
ATOM	1021	CG	LYS	1618	5.734	-3.465	-3.749	1.00	28.34
ATOM	1022	CD	LYS	1618	5.557	-4.914	-3.328	1.00	32.45
ATOM	1023	CE	LYS	1618	5.590	-5.850	-4.520	1.00	30.41
ATOM	1024	NZ	LYS	1618	4.373	-5.748	-5.354	1.00	31.84
ATOM	1025	C	LYS	1618	7.404	-1.610	-0.796	1.00	23.84
ATOM	1026	O	LYS	1618	7.533	-0.548	-1.402	1.00	20.60
ATOM	1027	N	CYS	1619	7.719	-1.744	0.489	1.00	25.11
ATOM	1028	CA	CYS	1619	8.103	-0.614	1.312	1.00	21.68
ATOM	1029	CB	CYS	1619	7.338	-0.690	2.643	1.00	20.84
ATOM	1030	SG	CYS	1619	7.916	0.427	3.957	1.00	26.69
ATOM	1031	C	CYS	1619	9.586	-0.480	1.543	1.00	23.16
ATOM	1032	O	CYS	1619	10.257	-1.435	1.958	1.00	25.60
ATOM	1033	N	ILE	1620	10.110	0.717	1.288	1.00	23.91
ATOM	1034	CA	ILE	1620	11.532	1.046	1.474	1.00	26.01

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ATOM	1035	CB	ILE	1620	12.098	1.830	0.236	1.00	22.61
ATOM	1036	CG2	ILE	1620	13.551	2.259	0.471	1.00	16.86
ATOM	1037	CG1	ILE	1620	12.014	0.977	-1.026	1.00	22.72
ATOM	1038	CD1	ILE	1620	12.096	1.804	-2.316	1.00	23.62
ATOM	1039	C	ILE	1620	11.566	1.934	2.729	1.00	26.83
ATOM	1040	O	ILE	1620	10.900	2.965	2.772	1.00	28.92
ATOM	1041	N	HIS	1621	12.293	1.500	3.758	1.00	26.44
ATOM	1042	CA	HIS	1621	12.386	2.245	5.007	1.00	23.61
ATOM	1043	CB	HIS	1621	13.142	1.429	6.065	1.00	20.98
ATOM	1044	CG	HIS	1621	12.940	1.917	7.463	1.00	21.57
ATOM	1045	CD2	HIS	1621	12.321	1.346	8.528	1.00	20.74
ATOM	1046	ND1	HIS	1621	13.382	3.151	7.897	1.00	21.08
ATOM	1047	CE1	HIS	1621	13.035	3.321	9.162	1.00	21.00
ATOM	1048	NE2	HIS	1621	12.396	2.237	9.572	1.00	21.97
ATOM	1049	C	HIS	1621	13.054	3.582	4.841	1.00	24.83
ATOM	1050	O	HIS	1621	12.560	4.585	5.310	1.00	25.76
ATOM	1051	N	ARG	1622	14.247	3.565	4.269	1.00	27.57
ATOM	1052	CA	ARG	1622	15.056	4.776	4.066	1.00	26.47
ATOM	1053	CB	ARG	1622	14.233	5.918	3.460	1.00	20.08
ATOM	1054	CG	ARG	1622	13.762	5.634	2.077	1.00	15.87
ATOM	1055	CD	ARG	1622	12.998	6.791	1.501	0.50	11.86
ATOM	1056	NE	ARG	1622	12.613	6.458	0.144	0.50	12.46
ATOM	1057	CZ	ARG	1622	11.537	5.748	-0.178	0.50	11.18
ATOM	1058	NH1	ARG	1622	10.711	5.304	0.767	0.50	7.16
ATOM	1059	NH2	ARG	1622	11.340	5.398	-1.442	0.50	9.57
ATOM	1060	C	ARG	1622	15.813	5.250	5.325	1.00	26.18
ATOM	1061	O	ARG	1622	16.645	6.150	5.250	1.00	26.90
ATOM	1062	N	ASP	1623	15.544	4.650	6.480	1.00	27.26
ATOM	1063	CA	ASP	1623	16.268	5.042	7.684	1.00	29.80
ATOM	1064	CB	ASP	1623	15.714	6.330	8.292	1.00	32.13
ATOM	1065	CG	ASP	1623	16.690	6.940	9.298	1.00	37.87
ATOM	1066	OD1	ASP	1623	16.237	7.671	10.202	1.00	42.95
ATOM	1067	OD2	ASP	1623	17.907	6.684	9.191	1.00	41.09
ATOM	1068	C	ASP	1623	16.364	3.943	8.738	1.00	29.10
ATOM	1069	O	ASP	1623	16.164	4.168	9.939	1.00	27.69
ATOM	1070	N	LEU	1624	16.723	2.755	8.270	1.00	28.23
ATOM	1071	CA	LEU	1624	16.874	1.599	9.129	1.00	26.00
ATOM	1072	CB	LEU	1624	16.944	0.351	8.245	1.00	22.14
ATOM	1073	CG	LEU	1624	17.036	-0.998	8.941	1.00	22.32
ATOM	1074	CD1	LEU	1624	15.853	-1.196	9.932	1.00	17.01
ATOM	1075	CD2	LEU	1624	17.068	-2.064	7.848	1.00	20.50
ATOM	1076	C	LEU	1624	18.129	1.757	10.003	1.00	25.89
ATOM	1077	O	LEU	1624	19.247	1.917	9.499	1.00	26.11
ATOM	1078	N	ALA	1625	17.930	1.706	11.316	1.00	25.58
ATOM	1079	CA	ALA	1625	19.006	1.864	12.292	1.00	23.16
ATOM	1080	CB	ALA	1625	19.323	3.340	12.493	1.00	19.06
ATOM	1081	C	ALA	1625	18.475	1.286	13.584	1.00	24.12
ATOM	1082	O	ALA	1625	17.269	1.083	13.721	1.00	27.40
ATOM	1083	N	ALA	1626	19.357	1.041	14.543	1.00	24.67
ATOM	1084	CA	ALA	1626	18.929	0.491	15.827	1.00	25.07
ATOM	1085	CB	ALA	1626	20.148	0.145	16.691	1.00	26.06
ATOM	1086	C	ALA	1626	18.015	1.474	16.560	1.00	25.13

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ATOM	1087	O	ALA	1626	17.184	1.069	17.366	1.00	26.38
ATOM	1088	N	ARG	1627	18.197	2.770	16.308	1.00	23.08
ATOM	1089	CA	ARG	1627	17.367	3.784	16.939	1.00	24.05
ATOM	1090	CB	ARG	1627	17.850	5.187	16.565	1.00	28.05
ATOM	1091	CG	ARG	1627	17.731	5.501	15.078	1.00	37.58
ATOM	1092	CD	ARG	1627	18.159	6.920	14.740	1.00	42.10
ATOM	1093	NE	ARG	1627	18.448	7.085	13.310	1.00	42.67
ATOM	1094	CZ	ARG	1627	19.667	7.006	12.784	1.00	43.58
ATOM	1095	NH1	ARG	1627	20.717	6.752	13.561	1.00	46.17
ATOM	1096	NH2	ARG	1627	19.841	7.201	11.492	1.00	43.78
ATOM	1097	C	ARG	1627	15.926	3.632	16.482	1.00	23.04
ATOM	1098	O	ARG	1627	15.015	3.979	17.216	1.00	22.27
ATOM	1099	N	ASN	1628	15.722	3.093	15.286	1.00	24.49
ATOM	1100	CA	ASN	1628	14.382	2.934	14.723	1.00	23.80
ATOM	1101	CB	ASN	1628	14.351	3.407	13.269	1.00	27.82
ATOM	1102	CG	ASN	1628	14.503	4.918	13.143	1.00	30.25
ATOM	1103	OD1	ASN	1628	13.876	5.686	13.863	1.00	32.33
ATOM	1104	ND2	ASN	1628	15.361	5.348	12.220	1.00	31.50
ATOM	1105	C	ASN	1628	13.782	1.524	14.833	1.00	23.93
ATOM	1106	O	ASN	1628	12.896	1.161	14.056	1.00	23.64
ATOM	1107	N	VAL	1629	14.307	0.733	15.763	1.00	24.10
ATOM	1108	CA	VAL	1629	13.778	-0.610	16.036	1.00	22.59
ATOM	1109	CB	VAL	1629	14.829	-1.727	15.823	1.00	21.16
ATOM	1110	CG1	VAL	1629	14.346	-3.014	16.462	1.00	17.53
ATOM	1111	CG2	VAL	1629	15.068	-1.962	14.341	1.00	14.48
ATOM	1112	C	VAL	1629	13.411	-0.575	17.520	1.00	24.81
ATOM	1113	O	VAL	1629	14.237	-0.204	18.357	1.00	24.09
ATOM	1114	N	LEU	1630	12.181	-0.941	17.850	1.00	24.34
ATOM	1115	CA	LEU	1630	11.751	-0.919	19.239	1.00	26.53
ATOM	1116	CB	LEU	1630	10.447	-0.129	19.359	1.00	26.19
ATOM	1117	CG	LEU	1630	10.522	1.293	18.758	1.00	24.33
ATOM	1118	CD1	LEU	1630	9.149	1.870	18.601	1.00	20.51
ATOM	1119	CD2	LEU	1630	11.339	2.196	19.618	1.00	19.77
ATOM	1120	C	LEU	1630	11.641	-2.327	19.835	1.00	28.14
ATOM	1121	O	LEU	1630	11.475	-3.320	19.108	1.00	28.31
ATOM	1122	N	VAL	1631	11.792	-2.418	21.153	1.00	28.21
ATOM	1123	CA	VAL	1631	11.741	-3.694	21.866	1.00	26.96
ATOM	1124	CB	VAL	1631	13.068	-3.930	22.624	1.00	25.71
ATOM	1125	CG1	VAL	1631	13.113	-5.345	23.222	1.00	20.40
ATOM	1126	CG2	VAL	1631	14.240	-3.688	21.680	1.00	19.88
ATOM	1127	C	VAL	1631	10.560	-3.758	22.836	1.00	29.84
ATOM	1128	O	VAL	1631	10.419	-2.918	23.738	1.00	32.46
ATOM	1129	N	THR	1632	9.703	-4.756	22.641	1.00	30.90
ATOM	1130	CA	THR	1632	8.530	-4.939	23.487	1.00	31.16
ATOM	1131	CB	THR	1632	7.476	-5.800	22.793	1.00	29.58
ATOM	1132	OG1	THR	1632	7.948	-7.152	22.708	1.00	29.17
ATOM	1133	CG2	THR	1632	7.186	-5.262	21.414	1.00	22.23
ATOM	1134	C	THR	1632	8.882	-5.603	24.809	1.00	32.23
ATOM	1135	O	THR	1632	9.950	-6.185	24.946	1.00	33.23
ATOM	1136	N	GLU	1633	7.946	-5.589	25.751	1.00	34.38
ATOM	1137	CA	GLU	1633	8.165	-6.193	27.062	1.00	35.51
ATOM	1138	CB	GLU	1633	6.881	-6.114	27.899	1.00	35.48

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ATOM	1139	CG	GLU	1633	7.004	-6.685	29.309	1.00	45.16
ATOM	1140	CD	GLU	1633	8.070	-5.999	30.183	1.00	50.45
ATOM	1141	OE1	GLU	1633	8.174	-4.750	30.163	1.00	52.70
ATOM	1142	OE2	GLU	1633	8.789	-6.723	30.919	1.00	53.59
ATOM	1143	C	GLU	1633	8.624	-7.635	26.930	1.00	35.40
ATOM	1144	O	GLU	1633	9.387	-8.119	27.758	1.00	36.57
ATOM	1145	N	ASP	1634	8.204	-8.308	25.861	1.00	36.76
ATOM	1146	CA	ASP	1634	8.573	-9.709	25.662	1.00	37.95
ATOM	1147	CB	ASP	1634	7.435	-10.491	24.991	1.00	42.90
ATOM	1148	CG	ASP	1634	6.100	-10.315	25.706	1.00	49.06
ATOM	1149	OD1	ASP	1634	5.885	-10.957	26.759	1.00	50.95
ATOM	1150	OD2	ASP	1634	5.256	-9.544	25.197	1.00	53.92
ATOM	1151	C	ASP	1634	9.842	-9.882	24.840	1.00	36.05
ATOM	1152	O	ASP	1634	10.148	-10.988	24.414	1.00	34.95
ATOM	1153	N	ASN	1635	10.582	-8.787	24.655	1.00	36.53
ATOM	1154	CA	ASN	1635	11.833	-8.763	23.868	1.00	36.21
ATOM	1155	CB	ASN	1635	12.893	-9.692	24.471	1.00	37.91
ATOM	1156	CG	ASN	1635	13.335	-9.244	25.840	1.00	37.60
ATOM	1157	OD1	ASN	1635	13.496	-8.057	26.088	1.00	42.72
ATOM	1158	ND2	ASN	1635	13.525	-10.191	26.743	1.00	38.03
ATOM	1159	C	ASN	1635	11.641	-9.073	22.372	1.00	34.59
ATOM	1160	O	ASN	1635	12.431	-9.799	21.754	1.00	33.52
ATOM	1161	N	VAL	1636	10.557	-8.541	21.819	1.00	31.95
ATOM	1162	CA	VAL	1636	10.260	-8.722	20.415	1.00	28.92
ATOM	1163	CB	VAL	1636	8.743	-8.945	20.177	1.00	31.00
ATOM	1164	CG1	VAL	1636	8.451	-9.066	18.678	1.00	29.52
ATOM	1165	CG2	VAL	1636	8.289	-10.220	20.884	1.00	29.03
ATOM	1166	C	VAL	1636	10.725	-7.461	19.721	1.00	28.05
ATOM	1167	O	VAL	1636	10.432	-6.355	20.179	1.00	25.21
ATOM	1168	N	MET	1637	11.567	-7.637	18.707	1.00	28.78
ATOM	1169	CA	MET	1637	12.107	-6.539	17.927	1.00	27.29
ATOM	1170	CB	MET	1637	13.325	-7.008	17.138	1.00	27.97
ATOM	1171	CG	MET	1637	14.446	-7.576	17.982	1.00	29.31
ATOM	1172	SD	MET	1637	15.051	-6.440	19.245	1.00	29.58
ATOM	1173	CE	MET	1637	15.163	-7.542	20.648	1.00	23.51
ATOM	1174	C	MET	1637	11.033	-6.108	16.951	1.00	26.60
ATOM	1175	O	MET	1637	10.479	-6.951	16.244	1.00	26.60
ATOM	1176	N	LYS	1638	10.758	-4.805	16.893	1.00	24.35
ATOM	1177	CA	LYS	1638	9.745	-4.255	16.006	1.00	20.79
ATOM	1178	CB	LYS	1638	8.495	-3.883	16.793	1.00	18.95
ATOM	1179	CG	LYS	1638	7.723	-5.087	17.268	1.00	22.82
ATOM	1180	CD	LYS	1638	6.442	-4.699	17.969	1.00	25.49
ATOM	1181	CE	LYS	1638	5.560	-5.934	18.189	1.00	24.36
ATOM	1182	NZ	LYS	1638	4.892	-6.414	16.941	1.00	22.23
ATOM	1183	C	LYS	1638	10.254	-3.034	15.257	1.00	22.79
ATOM	1184	O	LYS	1638	10.613	-2.041	15.868	1.00	24.60
ATOM	1185	N	ILE	1639	10.259	-3.101	13.934	1.00	23.92
ATOM	1186	CA	ILE	1639	10.707	-1.984	13.113	1.00	24.22
ATOM	1187	CB	ILE	1639	10.925	-2.439	11.648	1.00	23.18
ATOM	1188	CG2	ILE	1639	11.270	-1.262	10.766	1.00	17.17
ATOM	1189	CG1	ILE	1639	12.068	-3.454	11.604	1.00	19.97
ATOM	1190	CD1	ILE	1639	11.975	-4.369	10.461	1.00	26.92

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ATOM	1191	C	ILE	1639	9.686	-0.846	13.173	1.00	25.63
ATOM	1192	O	ILE	1639	8.473	-1.075	13.042	1.00	26.20
ATOM	1193	N	ALA	1640	10.200	0.364	13.390	1.00	27.31
ATOM	1194	CA	ALA	1640	9.394	1.577	13.497	1.00	27.45
ATOM	1195	CB	ALA	1640	9.623	2.211	14.862	1.00	27.20
ATOM	1196	C	ALA	1640	9.720	2.595	12.411	1.00	27.87
ATOM	1197	O	ALA	1640	10.765	2.522	11.755	1.00	26.95
ATOM	1198	N	ASP	1641	8.815	3.551	12.237	1.00	29.66
ATOM	1199	CA	ASP	1641	8.952	4.631	11.259	1.00	31.25
ATOM	1200	CB	ASP	1641	10.096	5.581	11.646	1.00	33.40
ATOM	1201	CG	ASP	1641	9.713	6.551	12.771	1.00	33.86
ATOM	1202	OD1	ASP	1641	10.475	7.524	12.953	1.00	37.57
ATOM	1203	OD2	ASP	1641	8.684	6.355	13.470	1.00	29.83
ATOM	1204	C	ASP	1641	9.088	4.228	9.799	1.00	30.77
ATOM	1205	O	ASP	1641	9.526	5.022	8.966	1.00	29.52
ATOM	1206	N	PHE	1642	8.611	3.032	9.477	1.00	30.38
ATOM	1207	CA	PHE	1642	8.664	2.528	8.114	1.00	29.43
ATOM	1208	CB	PHE	1642	8.459	1.009	8.100	1.00	25.46
ATOM	1209	CG	PHE	1642	7.167	0.555	8.697	1.00	20.44
ATOM	1210	CD1	PHE	1642	6.002	0.547	7.942	1.00	22.76
ATOM	1211	CD2	PHE	1642	7.119	0.112	10.007	1.00	18.52
ATOM	1212	CE1	PHE	1642	4.796	0.094	8.485	1.00	25.55
ATOM	1213	CE2	PHE	1642	5.926	-0.341	10.559	1.00	21.76
ATOM	1214	CZ	PHE	1642	4.760	-0.352	9.802	1.00	24.94
ATOM	1215	C	PHE	1642	7.686	3.242	7.163	1.00	31.03
ATOM	1216	O	PHE	1642	7.946	3.330	5.975	1.00	35.19
ATOM	1217	N	GLY	1643	6.600	3.791	7.693	1.00	30.42
ATOM	1218	CA	GLY	1643	5.640	4.476	6.845	1.00	28.27
ATOM	1219	C	GLY	1643	5.736	5.991	6.874	1.00	28.46
ATOM	1220	O	GLY	1643	4.896	6.707	6.332	1.00	24.29
ATOM	1221	N	LEU	1644	6.816	6.471	7.458	1.00	31.65
ATOM	1222	CA	LEU	1644	7.077	7.890	7.601	1.00	36.03
ATOM	1223	CB	LEU	1644	8.363	8.058	8.389	1.00	32.41
ATOM	1224	CG	LEU	1644	8.321	9.137	9.446	1.00	35.30
ATOM	1225	CD1	LEU	1644	7.161	8.827	10.384	1.00	37.60
ATOM	1226	CD2	LEU	1644	9.663	9.186	10.190	1.00	36.62
ATOM	1227	C	LEU	1644	7.178	8.708	6.293	1.00	40.21
ATOM	1228	O	LEU	1644	7.770	8.267	5.312	1.00	40.65
ATOM	1229	N	ALA	1645	6.553	9.881	6.293	1.00	44.50
ATOM	1230	CA	ALA	1645	6.591	10.786	5.148	1.00	48.66
ATOM	1231	CB	ALA	1645	5.432	11.762	5.241	1.00	45.63
ATOM	1232	C	ALA	1645	7.935	11.545	5.173	1.00	51.32
ATOM	1233	O	ALA	1645	8.254	12.200	6.163	1.00	52.68
ATOM	1234	N	ALA	1646	8.727	11.444	4.107	1.00	52.77
ATOM	1235	CA	ALA	1646	10.023	12.121	4.077	1.00	54.73
ATOM	1236	CB	ALA	1646	11.108	11.194	4.646	1.00	55.34
ATOM	1237	C	ALA	1646	10.446	12.601	2.692	1.00	56.41
ATOM	1238	O	ALA	1646	10.430	11.823	1.740	1.00	57.76
ATOM	1239	N	ASP	1647	10.811	13.876	2.567	1.00	58.20
ATOM	1240	CA	ASP	1647	11.280	14.394	1.283	1.00	59.39
ATOM	1241	CB	ASP	1647	10.898	15.861	1.083	1.00	59.29
ATOM	1242	CG	ASP	1647	11.128	16.339	-0.356	1.00	60.67

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ATOM	1243	OD1	ASP	1647	12.110	15.908	-1.009	1.00	61.21
ATOM	1244	OD2	ASP	1647	10.337	17.173	-0.835	1.00	61.34
ATOM	1245	C	ASP	1647	12.793	14.236	1.273	1.00	60.16
ATOM	1246	O	ASP	1647	13.523	15.023	1.889	1.00	58.16
ATOM	1247	N	ILE	1648	13.248	13.209	0.562	1.00	61.28
ATOM	1248	CA	ILE	1648	14.658	12.878	0.439	1.00	62.12
ATOM	1249	CB	ILE	1648	14.848	11.626	-0.444	1.00	59.97
ATOM	1250	CG2	ILE	1648	14.023	10.469	0.131	1.00	58.26
ATOM	1251	CG1	ILE	1648	14.429	11.922	-1.883	1.00	55.69
ATOM	1252	CD1	ILE	1648	15.005	10.976	-2.890	1.00	54.38
ATOM	1253	C	ILE	1648	15.470	14.047	-0.127	1.00	65.02
ATOM	1254	O	ILE	1648	16.633	14.245	0.233	1.00	66.85
ATOM	1255	N	HIS	1649	14.844	14.839	-0.995	1.00	65.85
ATOM	1256	CA	HIS	1649	15.505	15.992	-1.589	1.00	66.73
ATOM	1257	CB	HIS	1649	14.859	16.358	-2.934	1.00	65.67
ATOM	1258	CG	HIS	1649	15.142	15.388	-4.038	1.00	66.47
ATOM	1259	CD2	HIS	1649	16.253	14.686	-4.355	1.00	67.11
ATOM	1260	ND1	HIS	1649	14.210	15.064	-4.999	1.00	65.21
ATOM	1261	CE1	HIS	1649	14.733	14.216	-5.867	1.00	66.52
ATOM	1262	NE2	HIS	1649	15.974	13.966	-5.494	1.00	66.25
ATOM	1263	C	HIS	1649	15.505	17.200	-0.663	1.00	68.55
ATOM	1264	O	HIS	1649	15.636	18.341	-1.116	1.00	69.35
ATOM	1265	N	HIS	1650	15.273	16.963	0.629	1.00	71.25
ATOM	1266	CA	HIS	1650	15.262	18.026	1.633	1.00	73.53
ATOM	1267	CB	HIS	1650	13.849	18.551	1.860	1.00	76.79
ATOM	1268	CG	HIS	1650	13.342	19.448	0.765	1.00	83.36
ATOM	1269	CD2	HIS	1650	13.509	20.772	0.537	1.00	86.47
ATOM	1270	ND1	HIS	1650	12.571	18.984	-0.270	1.00	87.02
ATOM	1271	CE1	HIS	1650	12.279	19.983	-1.076	1.00	88.66
ATOM	1272	NE2	HIS	1650	12.840	21.080	-0.609	1.00	88.34
ATOM	1273	C	HIS	1650	15.872	17.580	2.965	1.00	73.11
ATOM	1274	O	HIS	1650	15.686	18.241	3.977	1.00	73.23
ATOM	1275	N	ILE	1651	16.599	16.464	2.949	1.00	72.64
ATOM	1276	CA	ILE	1651	17.234	15.937	4.143	1.00	72.54
ATOM	1277	CB	ILE	1651	17.660	14.472	3.942	1.00	74.59
ATOM	1278	CG2	ILE	1651	18.463	13.966	5.142	1.00	75.52
ATOM	1279	CG1	ILE	1651	16.426	13.591	3.752	1.00	77.59
ATOM	1280	CD1	ILE	1651	16.747	12.141	3.472	1.00	80.12
ATOM	1281	C	ILE	1651	18.463	16.769	4.523	1.00	71.47
ATOM	1282	O	ILE	1651	19.326	17.022	3.688	1.00	72.40
ATOM	1283	N	ASP	1652	18.529	17.197	5.784	1.00	70.34
ATOM	1284	CA	ASP	1652	19.678	17.976	6.235	1.00	68.57
ATOM	1285	CB	ASP	1652	19.272	18.878	7.411	1.00	72.80
ATOM	1286	CG	ASP	1652	20.456	19.640	7.982	1.00	76.90
ATOM	1287	OD1	ASP	1652	21.463	19.888	7.287	1.00	79.62
ATOM	1288	OD2	ASP	1652	20.369	20.030	9.170	1.00	80.36
ATOM	1289	C	ASP	1652	20.771	17.007	6.652	1.00	66.01
ATOM	1290	O	ASP	1652	20.709	16.421	7.735	1.00	64.75
ATOM	1291	N	TYR	1653	21.778	16.868	5.808	1.00	64.05
ATOM	1292	CA	TYR	1653	22.906	15.978	6.074	1.00	63.55
ATOM	1293	CB	TYR	1653	23.829	15.913	4.855	1.00	63.81
ATOM	1294	CG	TYR	1653	23.316	14.993	3.771	1.00	65.65

ATOM	1295	CD1	TYR	1653	24.082	14.710	2.643	1.00	65.32
ATOM	1296	CE1	TYR	1653	23.638	13.810	1.674	1.00	68.40
ATOM	1297	CD2	TYR	1653	22.079	14.357	3.903	1.00	66.72
ATOM	1298	CE2	TYR	1653	21.626	13.451	2.940	1.00	69.93
ATOM	1299	CZ	TYR	1653	22.409	13.182	1.833	1.00	70.13
ATOM	1300	OH	TYR	1653	21.966	12.272	0.902	1.00	72.73
ATOM	1301	C	TYR	1653	23.708	16.334	7.328	1.00	62.96
ATOM	1302	O	TYR	1653	24.342	15.473	7.938	1.00	63.31
ATOM	1303	N	TYR	1654	23.653	17.598	7.727	1.00	63.02
ATOM	1304	CA	TYR	1654	24.379	18.065	8.902	1.00	63.89
ATOM	1305	CB	TYR	1654	24.896	19.491	8.684	1.00	60.37
ATOM	1306	CG	TYR	1654	26.012	19.565	7.669	1.00	59.33
ATOM	1307	CD1	TYR	1654	25.735	19.673	6.313	1.00	59.29
ATOM	1308	CE1	TYR	1654	26.759	19.687	5.362	1.00	61.50
ATOM	1309	CD2	TYR	1654	27.349	19.480	8.061	1.00	60.05
ATOM	1310	CE2	TYR	1654	28.384	19.498	7.119	1.00	61.35
ATOM	1311	CZ	TYR	1654	28.082	19.598	5.773	1.00	62.41
ATOM	1312	OH	TYR	1654	29.098	19.589	4.842	1.00	60.57
ATOM	1313	C	TYR	1654	23.586	17.984	10.192	1.00	65.65
ATOM	1314	O	TYR	1654	24.104	18.321	11.252	1.00	67.31
ATOM	1315	N	LYS	1655	22.349	17.504	10.118	1.00	67.52
ATOM	1316	CA	LYS	1655	21.499	17.390	11.303	1.00	69.54
ATOM	1317	CB	LYS	1655	20.028	17.445	10.893	1.00	71.09
ATOM	1318	CG	LYS	1655	19.057	17.518	12.049	1.00	73.08
ATOM	1319	CD	LYS	1655	17.648	17.713	11.531	1.00	76.73
ATOM	1320	CE	LYS	1655	16.624	17.320	12.568	1.00	81.94
ATOM	1321	NZ	LYS	1655	15.232	17.521	12.072	1.00	84.53
ATOM	1322	C	LYS	1655	21.783	16.102	12.076	1.00	70.33
ATOM	1323	O	LYS	1655	21.952	15.032	11.478	1.00	70.43
ATOM	1324	N	LYS	1656	21.825	16.218	13.403	1.00	70.11
ATOM	1325	CA	LYS	1656	22.093	15.079	14.274	1.00	70.03
ATOM	1326	CB	LYS	1656	23.049	15.481	15.394	1.00	67.72
ATOM	1327	CG	LYS	1656	24.473	15.716	14.947	1.00	66.34
ATOM	1328	CD	LYS	1656	25.326	16.124	16.136	1.00	66.60
ATOM	1329	CE	LYS	1656	26.801	15.839	15.905	1.00	64.71
ATOM	1330	NZ	LYS	1656	27.612	16.059	17.138	1.00	62.24
ATOM	1331	C	LYS	1656	20.823	14.480	14.881	1.00	70.67
ATOM	1332	O	LYS	1656	19.759	15.104	14.864	1.00	71.91
ATOM	1333	N	THR	1657	20.941	13.265	15.412	1.00	69.38
ATOM	1334	CA	THR	1657	19.818	12.586	16.035	1.00	68.30
ATOM	1335	CB	THR	1657	20.052	11.051	16.101	1.00	69.30
ATOM	1336	OG1	THR	1657	21.179	10.757	16.941	1.00	68.20
ATOM	1337	CG2	THR	1657	20.310	10.479	14.713	1.00	69.71
ATOM	1338	C	THR	1657	19.706	13.145	17.445	1.00	67.60
ATOM	1339	O	THR	1657	20.521	13.971	17.846	1.00	67.40
ATOM	1340	N	ALA	1658	18.715	12.694	18.206	1.00	67.83
ATOM	1341	CA	ALA	1658	18.564	13.163	19.582	1.00	67.73
ATOM	1342	CB	ALA	1658	17.345	12.503	20.234	1.00	68.87
ATOM	1343	C	ALA	1658	19.833	12.820	20.364	1.00	66.59
ATOM	1344	O	ALA	1658	20.368	13.640	21.115	1.00	66.33
ATOM	1345	N	ASN	1659	20.343	11.616	20.129	1.00	65.38
ATOM	1346	CA	ASN	1659	21.545	11.143	20.801	1.00	62.65

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ATOM	1347	CB	ASN	1659	21.702	9.638	20.616	1.00	63.61
ATOM	1348	CG	ASN	1659	22.548	9.009	21.697	1.00	64.09
ATOM	1349	OD1	ASN	1659	22.526	9.451	22.850	1.00	63.69
ATOM	1350	ND2	ASN	1659	23.279	7.959	21.345	1.00	64.10
ATOM	1351	C	ASN	1659	22.808	11.844	20.321	1.00	60.46
ATOM	1352	O	ASN	1659	23.882	11.601	20.856	1.00	60.78
ATOM	1353	N	GLY	1660	22.671	12.675	19.285	1.00	58.84
ATOM	1354	CA	GLY	1660	23.803	13.407	18.735	1.00	56.69
ATOM	1355	C	GLY	1660	24.570	12.721	17.616	1.00	56.40
ATOM	1356	O	GLY	1660	25.738	13.028	17.377	1.00	56.43
ATOM	1357	N	ARG	1661	23.929	11.779	16.937	1.00	56.00
ATOM	1358	CA	ARG	1661	24.585	11.048	15.849	1.00	53.80
ATOM	1359	CB	ARG	1661	24.312	9.540	15.952	1.00	54.52
ATOM	1360	CG	ARG	1661	24.876	8.879	17.218	1.00	55.28
ATOM	1361	CD	ARG	1661	24.556	7.395	17.226	1.00	58.01
ATOM	1362	NE	ARG	1661	25.051	6.670	18.396	1.00	58.41
ATOM	1363	CZ	ARG	1661	24.918	5.355	18.559	1.00	59.08
ATOM	1364	NH1	ARG	1661	24.306	4.637	17.623	1.00	55.82
ATOM	1365	NH2	ARG	1661	25.394	4.762	19.652	1.00	57.53
ATOM	1366	C	ARG	1661	24.139	11.581	14.491	1.00	51.03
ATOM	1367	O	ARG	1661	23.160	12.323	14.401	1.00	48.69
ATOM	1368	N	LEU	1662	24.859	11.189	13.440	1.00	48.33
ATOM	1369	CA	LEU	1662	24.565	11.647	12.087	1.00	45.87
ATOM	1370	CB	LEU	1662	25.839	12.199	11.426	1.00	46.18
ATOM	1371	CG	LEU	1662	26.374	13.511	12.016	1.00	45.78
ATOM	1372	CD1	LEU	1662	27.856	13.681	11.722	1.00	45.92
ATOM	1373	CD2	LEU	1662	25.576	14.698	11.489	1.00	44.92
ATOM	1374	C	LEU	1662	23.961	10.542	11.230	1.00	43.02
ATOM	1375	O	LEU	1662	24.647	9.607	10.811	1.00	42.04
ATOM	1376	N	PRO	1663	22.648	10.640	10.968	1.00	41.48
ATOM	1377	CD	PRO	1663	21.769	11.718	11.468	1.00	40.54
ATOM	1378	CA	PRO	1663	21.886	9.680	10.161	1.00	39.60
ATOM	1379	CB	PRO	1663	20.582	10.424	9.889	1.00	38.77
ATOM	1380	CG	PRO	1663	20.386	11.183	11.151	1.00	40.83
ATOM	1381	C	PRO	1663	22.578	9.273	8.860	1.00	35.90
ATOM	1382	O	PRO	1663	22.448	8.124	8.427	1.00	36.85
ATOM	1383	N	VAL	1664	23.356	10.180	8.276	1.00	33.16
ATOM	1384	CA	VAL	1664	24.053	9.880	7.024	1.00	32.51
ATOM	1385	CB	VAL	1664	24.851	11.106	6.439	1.00	32.44
ATOM	1386	CG1	VAL	1664	23.917	12.213	6.065	1.00	26.99
ATOM	1387	CG2	VAL	1664	25.897	11.607	7.421	1.00	29.84
ATOM	1388	C	VAL	1664	24.989	8.675	7.158	1.00	30.30
ATOM	1389	O	VAL	1664	25.400	8.091	6.161	1.00	30.16
ATOM	1390	N	LYS	1665	25.278	8.276	8.393	1.00	27.72
ATOM	1391	CA	LYS	1665	26.170	7.151	8.649	1.00	27.96
ATOM	1392	CB	LYS	1665	26.808	7.276	10.025	1.00	26.42
ATOM	1393	CG	LYS	1665	27.857	8.351	10.061	1.00	28.20
ATOM	1394	CD	LYS	1665	28.221	8.754	11.478	1.00	32.47
ATOM	1395	CE	LYS	1665	29.398	9.720	11.468	1.00	32.33
ATOM	1396	NZ	LYS	1665	29.713	10.231	12.819	1.00	30.38
ATOM	1397	C	LYS	1665	25.522	5.794	8.486	1.00	25.81
ATOM	1398	O	LYS	1665	26.159	4.769	8.691	1.00	27.53

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ATOM	1399	N	TRP	1666	24.247	5.793	8.120	1.00	26.13
ATOM	1400	CA	TRP	1666	23.499	4.554	7.896	1.00	25.88
ATOM	1401	CB	TRP	1666	22.259	4.537	8.800	1.00	26.15
ATOM	1402	CG	TRP	1666	22.547	4.067	10.226	1.00	28.12
ATOM	1403	CD2	TRP	1666	23.020	4.864	11.324	1.00	26.14
ATOM	1404	CE2	TRP	1666	23.154	4.009	12.438	1.00	24.97
ATOM	1405	CE3	TRP	1666	23.349	6.225	11.475	1.00	25.14
ATOM	1406	CD1	TRP	1666	22.408	2.795	10.715	1.00	26.09
ATOM	1407	NE1	TRP	1666	22.777	2.751	12.034	1.00	22.55
ATOM	1408	CZ2	TRP	1666	23.606	4.453	13.684	1.00	25.32
ATOM	1409	CZ3	TRP	1666	23.795	6.664	12.712	1.00	21.72
ATOM	1410	CH2	TRP	1666	23.920	5.782	13.798	1.00	23.77
ATOM	1411	C	TRP	1666	23.092	4.444	6.425	1.00	24.79
ATOM	1412	O	TRP	1666	22.662	3.390	5.971	1.00	25.26
ATOM	1413	N	MET	1667	23.350	5.508	5.664	1.00	24.21
ATOM	1414	CA	MET	1667	22.963	5.568	4.252	1.00	23.79
ATOM	1415	CB	MET	1667	22.796	7.018	3.809	1.00	25.08
ATOM	1416	CG	MET	1667	21.793	7.813	4.564	1.00	32.58
ATOM	1417	SD	MET	1667	21.778	9.495	3.910	1.00	41.43
ATOM	1418	CE	MET	1667	21.011	9.209	2.387	1.00	40.85
ATOM	1419	C	MET	1667	23.938	4.942	3.279	1.00	22.52
ATOM	1420	O	MET	1667	25.139	5.173	3.362	1.00	23.63
ATOM	1421	N	ALA	1668	23.406	4.195	2.324	1.00	22.77
ATOM	1422	CA	ALA	1668	24.218	3.576	1.278	1.00	24.91
ATOM	1423	CB	ALA	1668	23.342	2.672	0.396	1.00	24.41
ATOM	1424	C	ALA	1668	24.800	4.706	0.438	1.00	26.66
ATOM	1425	O	ALA	1668	24.163	5.748	0.251	1.00	24.54
ATOM	1426	N	PRO	1669	26.011	4.511	-0.101	1.00	26.97
ATOM	1427	CD	PRO	1669	26.935	3.374	0.066	1.00	26.23
ATOM	1428	CA	PRO	1669	26.614	5.563	-0.919	1.00	26.05
ATOM	1429	CB	PRO	1669	27.855	4.876	-1.482	1.00	24.03
ATOM	1430	CG	PRO	1669	28.259	3.946	-0.358	1.00	26.27
ATOM	1431	C	PRO	1669	25.687	6.048	-2.030	1.00	26.44
ATOM	1432	O	PRO	1669	25.576	7.250	-2.263	1.00	27.72
ATOM	1433	N	GLU	1670	24.971	5.137	-2.685	1.00	27.16
ATOM	1434	CA	GLU	1670	24.093	5.553	-3.769	1.00	27.63
ATOM	1435	CB	GLU	1670	23.613	4.365	-4.614	1.00	29.35
ATOM	1436	CG	GLU	1670	22.545	3.492	-3.980	1.00	29.16
ATOM	1437	CD	GLU	1670	23.089	2.238	-3.310	1.00	28.03
ATOM	1438	OE1	GLU	1670	22.248	1.430	-2.874	1.00	24.12
ATOM	1439	OE2	GLU	1670	24.325	2.040	-3.215	1.00	26.07
ATOM	1440	C	GLU	1670	22.931	6.407	-3.301	1.00	25.52
ATOM	1441	O	GLU	1670	22.477	7.281	-4.042	1.00	24.12
ATOM	1442	N	ALA	1671	22.452	6.163	-2.084	1.00	27.74
ATOM	1443	CA	ALA	1671	21.337	6.928	-1.510	1.00	27.65
ATOM	1444	CB	ALA	1671	20.729	6.189	-0.319	1.00	23.18
ATOM	1445	C	ALA	1671	21.860	8.283	-1.065	1.00	28.22
ATOM	1446	O	ALA	1671	21.234	9.310	-1.305	1.00	28.51
ATOM	1447	N	LEU	1672	23.011	8.266	-0.406	1.00	30.60
ATOM	1448	CA	LEU	1672	23.647	9.484	0.074	1.00	32.67
ATOM	1449	CB	LEU	1672	24.831	9.127	0.952	1.00	32.05
ATOM	1450	CG	LEU	1672	25.662	10.264	1.527	1.00	34.00

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ATOM	1451	CD1	LEU	1672	24.874	10.981	2.577	1.00	38.85
ATOM	1452	CD2	LEU	1672	26.910	9.667	2.149	1.00	35.22
ATOM	1453	C	LEU	1672	24.121	10.398	-1.067	1.00	37.10
ATOM	1454	O	LEU	1672	23.799	11.580	-1.086	1.00	37.19
ATOM	1455	N	PHE	1673	24.905	9.858	-1.997	1.00	37.60
ATOM	1456	CA	PHE	1673	25.403	10.664	-3.102	1.00	37.11
ATOM	1457	CB	PHE	1673	26.692	10.061	-3.667	1.00	35.24
ATOM	1458	CG	PHE	1673	27.782	9.857	-2.644	1.00	33.54
ATOM	1459	CD1	PHE	1673	28.456	8.633	-2.566	1.00	31.54
ATOM	1460	CD2	PHE	1673	28.143	10.874	-1.762	1.00	33.10
ATOM	1461	CE1	PHE	1673	29.467	8.421	-1.623	1.00	34.66
ATOM	1462	CE2	PHE	1673	29.156	10.678	-0.816	1.00	35.41
ATOM	1463	CZ	PHE	1673	29.819	9.444	-0.748	1.00	34.81
ATOM	1464	C	PHE	1673	24.406	10.890	-4.245	1.00	39.03
ATOM	1465	O	PHE	1673	24.276	11.997	-4.734	1.00	39.02
ATOM	1466	N	ASP	1674	23.693	9.844	-4.651	1.00	42.35
ATOM	1467	CA	ASP	1674	22.757	9.931	-5.762	1.00	41.59
ATOM	1468	CB	ASP	1674	22.957	8.736	-6.700	1.00	46.08
ATOM	1469	CG	ASP	1674	24.384	8.617	-7.201	1.00	51.20
ATOM	1470	OD1	ASP	1674	25.057	9.663	-7.333	1.00	53.97
ATOM	1471	OD2	ASP	1674	24.822	7.470	-7.469	1.00	50.65
ATOM	1472	C	ASP	1674	21.263	9.999	-5.418	1.00	42.89
ATOM	1473	O	ASP	1674	20.427	10.079	-6.317	1.00	41.95
ATOM	1474	N	ARG	1675	20.923	9.899	-4.134	1.00	42.82
ATOM	1475	CA	ARG	1675	19.521	9.944	-3.706	1.00	42.64
ATOM	1476	CB	ARG	1675	18.890	11.300	-4.028	1.00	48.80
ATOM	1477	CG	ARG	1675	19.480	12.449	-3.252	1.00	61.19
ATOM	1478	CD	ARG	1675	19.407	13.727	-4.068	1.00	72.90
ATOM	1479	NE	ARG	1675	20.025	14.854	-3.381	1.00	83.15
ATOM	1480	CZ	ARG	1675	19.652	16.123	-3.539	1.00	88.21
ATOM	1481	NH1	ARG	1675	18.662	16.439	-4.365	1.00	89.58
ATOM	1482	NH2	ARG	1675	20.265	17.085	-2.860	1.00	92.07
ATOM	1483	C	ARG	1675	18.674	8.825	-4.299	1.00	38.05
ATOM	1484	O	ARG	1675	17.495	9.005	-4.588	1.00	38.87
ATOM	1485	N	ILE	1676	19.281	7.658	-4.479	1.00	34.44
ATOM	1486	CA	ILE	1676	18.576	6.514	-5.012	1.00	30.11
ATOM	1487	CB	ILE	1676	19.378	5.825	-6.096	1.00	29.58
ATOM	1488	CG2	ILE	1676	18.509	4.850	-6.797	1.00	30.72
ATOM	1489	CG1	ILE	1676	19.835	6.868	-7.116	1.00	34.29
ATOM	1490	CD1	ILE	1676	20.798	6.348	-8.145	1.00	41.15
ATOM	1491	C	ILE	1676	18.315	5.541	-3.874	1.00	26.90
ATOM	1492	O	ILE	1676	19.236	4.898	-3.364	1.00	22.06
ATOM	1493	N	TYR	1677	17.056	5.465	-3.454	1.00	28.17
ATOM	1494	CA	TYR	1677	16.677	4.589	-2.350	1.00	26.80
ATOM	1495	CB	TYR	1677	15.742	5.310	-1.398	1.00	26.05
ATOM	1496	CG	TYR	1677	16.442	6.367	-0.580	1.00	26.92
ATOM	1497	CD1	TYR	1677	16.510	7.693	-1.018	1.00	23.98
ATOM	1498	CE1	TYR	1677	17.129	8.665	-0.250	1.00	23.90
ATOM	1499	CD2	TYR	1677	17.022	6.048	0.644	1.00	26.99
ATOM	1500	CE2	TYR	1677	17.642	7.017	1.414	1.00	24.87
ATOM	1501	CZ	TYR	1677	17.685	8.315	0.968	1.00	26.44
ATOM	1502	OH	TYR	1677	18.227	9.273	1.783	1.00	30.89

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ATOM	1503	C	TYR	1677	16.006	3.350	-2.894	1.00	26.30
ATOM	1504	O	TYR	1677	15.080	3.445	-3.703	1.00	28.12
ATOM	1505	N	THR	1678	16.489	2.197	-2.458	1.00	25.46
ATOM	1506	CA	THR	1678	15.973	0.918	-2.927	1.00	26.27
ATOM	1507	CB	THR	1678	16.904	0.336	-3.994	1.00	28.43
ATOM	1508	OG1	THR	1678	18.185	0.095	-3.405	1.00	30.59
ATOM	1509	CG2	THR	1678	17.068	1.305	-5.174	1.00	26.56
ATOM	1510	C	THR	1678	15.987	-0.049	-1.758	1.00	24.60
ATOM	1511	O	THR	1678	16.476	0.277	-0.693	1.00	27.15
ATOM	1512	N	HIS	1679	15.500	-1.260	-1.974	1.00	23.23
ATOM	1513	CA	HIS	1679	15.496	-2.276	-0.933	1.00	21.51
ATOM	1514	CB	HIS	1679	14.747	-3.520	-1.411	1.00	20.84
ATOM	1515	CG	HIS	1679	13.297	-3.279	-1.695	1.00	21.48
ATOM	1516	CD2	HIS	1679	12.552	-3.476	-2.812	1.00	22.71
ATOM	1517	ND1	HIS	1679	12.423	-2.795	-0.741	1.00	27.21
ATOM	1518	CE1	HIS	1679	11.206	-2.713	-1.255	1.00	22.60
ATOM	1519	NE2	HIS	1679	11.255	-3.116	-2.515	1.00	23.66
ATOM	1520	C	HIS	1679	16.976	-2.591	-0.665	1.00	20.81
ATOM	1521	O	HIS	1679	17.358	-2.954	0.451	1.00	22.50
ATOM	1522	N	GLN	1680	17.799	-2.382	-1.695	1.00	19.58
ATOM	1523	CA	GLN	1680	19.248	-2.587	-1.657	1.00	20.89
ATOM	1524	CB	GLN	1680	19.860	-2.400	-3.038	1.00	23.76
ATOM	1525	CG	GLN	1680	19.896	-3.651	-3.877	1.00	34.08
ATOM	1526	CD	GLN	1680	19.015	-3.559	-5.096	1.00	37.77
ATOM	1527	OE1	GLN	1680	18.069	-2.780	-5.122	1.00	43.23
ATOM	1528	NE2	GLN	1680	19.321	-4.356	-6.113	1.00	37.02
ATOM	1529	C	GLN	1680	19.913	-1.609	-0.724	1.00	20.72
ATOM	1530	O	GLN	1680	20.814	-1.981	0.021	1.00	21.53
ATOM	1531	N	SER	1681	19.514	-0.350	-0.773	1.00	21.01
ATOM	1532	CA	SER	1681	20.128	0.606	0.135	1.00	23.86
ATOM	1533	CB	SER	1681	19.841	2.065	-0.248	1.00	21.10
ATOM	1534	OG	SER	1681	18.473	2.290	-0.506	1.00	23.18
ATOM	1535	C	SER	1681	19.695	0.292	1.564	1.00	23.91
ATOM	1536	O	SER	1681	20.457	0.542	2.495	1.00	26.70
ATOM	1537	N	ASP	1682	18.511	-0.303	1.739	1.00	21.71
ATOM	1538	CA	ASP	1682	18.044	-0.662	3.080	1.00	21.28
ATOM	1539	CB	ASP	1682	16.595	-1.149	3.070	1.00	23.22
ATOM	1540	CG	ASP	1682	15.569	-0.016	3.198	1.00	23.08
ATOM	1541	OD1	ASP	1682	14.363	-0.282	3.017	1.00	21.99
ATOM	1542	OD2	ASP	1682	15.948	1.135	3.498	1.00	24.42
ATOM	1543	C	ASP	1682	18.955	-1.756	3.611	1.00	20.86
ATOM	1544	O	ASP	1682	19.289	-1.770	4.799	1.00	21.62
ATOM	1545	N	VAL	1683	19.398	-2.649	2.727	1.00	21.60
ATOM	1546	CA	VAL	1683	20.307	-3.732	3.122	1.00	22.27
ATOM	1547	CB	VAL	1683	20.515	-4.740	1.965	1.00	22.22
ATOM	1548	CG1	VAL	1683	21.587	-5.777	2.315	1.00	21.52
ATOM	1549	CG2	VAL	1683	19.187	-5.437	1.662	1.00	20.89
ATOM	1550	C	VAL	1683	21.618	-3.150	3.666	1.00	21.96
ATOM	1551	O	VAL	1683	22.107	-3.577	4.705	1.00	24.39
ATOM	1552	N	TRP	1684	22.172	-2.160	2.970	1.00	22.01
ATOM	1553	CA	TRP	1684	23.375	-1.489	3.449	1.00	23.06
ATOM	1554	CB	TRP	1684	23.685	-0.273	2.566	1.00	20.25

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ATOM	1555	CG	TRP	1684	24.808	0.549	3.069	1.00	22.35
ATOM	1556	CD2	TRP	1684	26.118	0.644	2.503	1.00	24.14
ATOM	1557	CE2	TRP	1684	26.879	1.500	3.334	1.00	23.68
ATOM	1558	CE3	TRP	1684	26.728	0.091	1.370	1.00	25.09
ATOM	1559	CD1	TRP	1684	24.825	1.346	4.193	1.00	22.52
ATOM	1560	NE1	TRP	1684	26.066	1.915	4.355	1.00	21.48
ATOM	1561	CZ2	TRP	1684	28.216	1.815	3.061	1.00	20.56
ATOM	1562	CZ3	TRP	1684	28.059	0.405	1.095	1.00	23.92
ATOM	1563	CH2	TRP	1684	28.785	1.257	1.942	1.00	23.18
ATOM	1564	C	TRP	1684	23.105	-1.025	4.903	1.00	23.96
ATOM	1565	O	TRP	1684	23.889	-1.308	5.815	1.00	25.98
ATOM	1566	N	SER	1685	21.992	-0.332	5.118	1.00	24.68
ATOM	1567	CA	SER	1685	21.615	0.144	6.447	1.00	22.75
ATOM	1568	CB	SER	1685	20.266	0.870	6.376	1.00	21.11
ATOM	1569	OG	SER	1685	20.276	1.950	5.452	1.00	21.98
ATOM	1570	C	SER	1685	21.516	-1.011	7.457	1.00	23.06
ATOM	1571	O	SER	1685	21.865	-0.850	8.638	1.00	22.55
ATOM	1572	N	PHE	1686	21.041	-2.168	6.998	1.00	21.83
ATOM	1573	CA	PHE	1686	20.915	-3.340	7.854	1.00	21.92
ATOM	1574	CB	PHE	1686	20.153	-4.457	7.129	1.00	18.02
ATOM	1575	CG	PHE	1686	19.965	-5.683	7.971	1.00	20.86
ATOM	1576	CD1	PHE	1686	19.142	-5.641	9.108	1.00	18.76
ATOM	1577	CD2	PHE	1686	20.669	-6.853	7.688	1.00	18.96
ATOM	1578	CE1	PHE	1686	19.023	-6.743	9.947	1.00	19.29
ATOM	1579	CE2	PHE	1686	20.554	-7.965	8.514	1.00	19.27
ATOM	1580	CZ	PHE	1686	19.732	-7.908	9.653	1.00	21.91
ATOM	1581	C	PHE	1686	22.304	-3.845	8.316	1.00	22.11
ATOM	1582	O	PHE	1686	22.473	-4.378	9.436	1.00	21.35
ATOM	1583	N	GLY	1687	23.294	-3.691	7.436	1.00	20.48
ATOM	1584	CA	GLY	1687	24.653	-4.079	7.769	1.00	20.41
ATOM	1585	C	GLY	1687	25.185	-3.211	8.899	1.00	19.03
ATOM	1586	O	GLY	1687	25.857	-3.714	9.808	1.00	20.27
ATOM	1587	N	VAL	1688	24.893	-1.906	8.829	1.00	20.57
ATOM	1588	CA	VAL	1688	25.296	-0.937	9.860	1.00	21.14
ATOM	1589	CB	VAL	1688	24.974	0.548	9.467	1.00	20.78
ATOM	1590	CG1	VAL	1688	25.440	1.493	10.564	1.00	21.51
ATOM	1591	CG2	VAL	1688	25.681	0.923	8.186	1.00	19.70
ATOM	1592	C	VAL	1688	24.547	-1.297	11.142	1.00	23.16
ATOM	1593	O	VAL	1688	25.126	-1.271	12.225	1.00	24.14
ATOM	1594	N	LEU	1689	23.264	-1.648	11.021	1.00	24.50
ATOM	1595	CA	LEU	1689	22.465	-2.058	12.187	1.00	25.93
ATOM	1596	CB	LEU	1689	21.008	-2.316	11.776	1.00	25.42
ATOM	1597	CG	LEU	1689	19.933	-2.392	12.874	1.00	26.29
ATOM	1598	CD1	LEU	1689	18.572	-2.053	12.272	1.00	23.43
ATOM	1599	CD2	LEU	1689	19.885	-3.768	13.543	1.00	25.66
ATOM	1600	C	LEU	1689	23.080	-3.330	12.797	1.00	28.01
ATOM	1601	O	LEU	1689	23.203	-3.426	14.016	1.00	30.06
ATOM	1602	N	LEU	1690	23.487	-4.287	11.956	1.00	27.19
ATOM	1603	CA	LEU	1690	24.111	-5.520	12.457	1.00	25.29
ATOM	1604	CB	LEU	1690	24.556	-6.446	11.315	1.00	24.98
ATOM	1605	CG	LEU	1690	23.594	-7.390	10.589	1.00	24.85
ATOM	1606	CD1	LEU	1690	24.385	-8.132	9.538	1.00	24.22

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ATOM	1607	CD2	LEU	1690	22.960	-8.434	11.512	1.00	19.10
ATOM	1608	C	LEU	1690	25.326	-5.123	13.291	1.00	24.70
ATOM	1609	O	LEU	1690	25.521	-5.624	14.408	1.00	23.57
ATOM	1610	N	TRP	1691	26.117	-4.197	12.747	1.00	23.68
ATOM	1611	CA	TRP	1691	27.316	-3.693	13.425	1.00	24.83
ATOM	1612	CB	TRP	1691	27.998	-2.621	12.567	1.00	20.94
ATOM	1613	CG	TRP	1691	29.331	-2.173	13.105	1.00	24.80
ATOM	1614	CD2	TRP	1691	29.565	-1.082	14.004	1.00	23.71
ATOM	1615	CE2	TRP	1691	30.966	-0.996	14.208	1.00	23.81
ATOM	1616	CE3	TRP	1691	28.726	-0.167	14.652	1.00	22.20
ATOM	1617	CD1	TRP	1691	30.570	-2.702	12.811	1.00	24.44
ATOM	1618	NE1	TRP	1691	31.550	-1.995	13.471	1.00	25.38
ATOM	1619	CZ2	TRP	1691	31.543	-0.022	15.034	1.00	24.39
ATOM	1620	CZ3	TRP	1691	29.300	0.799	15.484	1.00	21.99
ATOM	1621	CH2	TRP	1691	30.700	0.862	15.665	1.00	25.57
ATOM	1622	C	TRP	1691	26.998	-3.131	14.823	1.00	25.87
ATOM	1623	O	TRP	1691	27.772	-3.301	15.750	1.00	27.39
ATOM	1624	N	GLU	1692	25.865	-2.448	14.956	1.00	26.45
ATOM	1625	CA	GLU	1692	25.452	-1.869	16.238	1.00	25.13
ATOM	1626	CB	GLU	1692	24.257	-0.933	16.068	1.00	23.56
ATOM	1627	CG	GLU	1692	24.365	0.091	14.962	1.00	18.73
ATOM	1628	CD	GLU	1692	23.111	0.935	14.880	1.00	23.79
ATOM	1629	OE1	GLU	1692	22.303	0.722	13.962	1.00	22.70
ATOM	1630	OE2	GLU	1692	22.919	1.819	15.738	1.00	25.63
ATOM	1631	C	GLU	1692	25.072	-2.963	17.225	1.00	25.28
ATOM	1632	O	GLU	1692	25.278	-2.818	18.422	1.00	27.65
ATOM	1633	N	ILE	1693	24.484	-4.046	16.720	1.00	26.23
ATOM	1634	CA	ILE	1693	24.080	-5.164	17.565	1.00	23.81
ATOM	1635	CB	ILE	1693	23.177	-6.203	16.787	1.00	22.99
ATOM	1636	CG2	ILE	1693	22.966	-7.465	17.637	1.00	21.67
ATOM	1637	CG1	ILE	1693	21.820	-5.569	16.416	1.00	20.23
ATOM	1638	CD1	ILE	1693	20.964	-6.395	15.435	1.00	13.67
ATOM	1639	C	ILE	1693	25.322	-5.843	18.133	1.00	24.77
ATOM	1640	O	ILE	1693	25.401	-6.126	19.324	1.00	24.94
ATOM	1641	N	PHE	1694	26.329	-6.051	17.304	1.00	27.59
ATOM	1642	CA	PHE	1694	27.503	-6.709	17.827	1.00	29.42
ATOM	1643	CB	PHE	1694	28.122	-7.623	16.771	1.00	29.37
ATOM	1644	CG	PHE	1694	27.142	-8.649	16.263	1.00	27.99
ATOM	1645	CD1	PHE	1694	26.522	-8.486	15.034	1.00	28.43
ATOM	1646	CD2	PHE	1694	26.751	-9.709	17.074	1.00	27.86
ATOM	1647	CE1	PHE	1694	25.525	-9.355	14.625	1.00	30.12
ATOM	1648	CE2	PHE	1694	25.751	-10.586	16.674	1.00	25.78
ATOM	1649	CZ	PHE	1694	25.136	-10.408	15.453	1.00	26.17
ATOM	1650	C	PHE	1694	28.495	-5.821	18.578	1.00	29.83
ATOM	1651	O	PHE	1694	29.485	-6.305	19.126	1.00	32.81
ATOM	1652	N	THR	1695	28.217	-4.516	18.635	1.00	28.35
ATOM	1653	CA	THR	1695	29.044	-3.598	19.419	1.00	25.39
ATOM	1654	CB	THR	1695	29.540	-2.379	18.627	1.00	21.81
ATOM	1655	OG1	THR	1695	28.422	-1.628	18.137	1.00	21.54
ATOM	1656	CG2	THR	1695	30.457	-2.816	17.508	1.00	16.93
ATOM	1657	C	THR	1695	28.198	-3.126	20.604	1.00	26.16
ATOM	1658	O	THR	1695	28.620	-2.268	21.386	1.00	26.77

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ATOM	1659	N	LEU	1696	27.023	-3.747	20.747	1.00	26.87
ATOM	1660	CA	LEU	1696	26.069	-3.446	21.813	1.00	27.64
ATOM	1661	CB	LEU	1696	26.572	-3.977	23.156	1.00	30.54
ATOM	1662	CG	LEU	1696	26.903	-5.456	23.182	1.00	29.75
ATOM	1663	CD1	LEU	1696	27.448	-5.821	24.546	1.00	32.53
ATOM	1664	CD2	LEU	1696	25.658	-6.234	22.882	1.00	33.79
ATOM	1665	C	LEU	1696	25.727	-1.984	21.946	1.00	25.51
ATOM	1666	O	LEU	1696	25.824	-1.410	23.025	1.00	27.90
ATOM	1667	N	GLY	1697	25.265	-1.395	20.857	1.00	26.48
ATOM	1668	CA	GLY	1697	24.899	0.007	20.859	1.00	25.81
ATOM	1669	C	GLY	1697	26.040	0.900	20.452	1.00	26.40
ATOM	1670	O	GLY	1697	26.055	2.090	20.760	1.00	29.69
ATOM	1671	N	GLY	1698	27.008	0.330	19.748	1.00	27.65
ATOM	1672	CA	GLY	1698	28.150	1.110	19.314	1.00	28.38
ATOM	1673	C	GLY	1698	27.795	2.186	18.310	1.00	30.13
ATOM	1674	O	GLY	1698	26.896	2.028	17.496	1.00	32.55
ATOM	1675	N	SER	1699	28.520	3.295	18.375	1.00	30.56
ATOM	1676	CA	SER	1699	28.304	4.420	17.491	1.00	32.11
ATOM	1677	CB	SER	1699	28.622	5.714	18.246	1.00	33.58
ATOM	1678	OG	SER	1699	28.578	6.863	17.407	1.00	38.87
ATOM	1679	C	SER	1699	29.203	4.269	16.268	1.00	32.10
ATOM	1680	O	SER	1699	30.408	4.073	16.403	1.00	31.12
ATOM	1681	N	PRO	1700	28.629	4.324	15.062	1.00	32.70
ATOM	1682	CD	PRO	1700	27.204	4.482	14.745	1.00	34.35
ATOM	1683	CA	PRO	1700	29.427	4.192	13.837	1.00	32.25
ATOM	1684	CB	PRO	1700	28.358	4.096	12.736	1.00	32.85
ATOM	1685	CG	PRO	1700	27.101	3.713	13.461	1.00	35.54
ATOM	1686	C	PRO	1700	30.258	5.456	13.651	1.00	31.84
ATOM	1687	O	PRO	1700	29.792	6.550	13.983	1.00	31.56
ATOM	1688	N	TYR	1701	31.487	5.306	13.170	1.00	31.07
ATOM	1689	CA	TYR	1701	32.372	6.441	12.910	1.00	32.41
ATOM	1690	CB	TYR	1701	32.039	7.055	11.537	1.00	32.39
ATOM	1691	CG	TYR	1701	32.088	6.092	10.378	1.00	35.63
ATOM	1692	CD1	TYR	1701	30.936	5.807	9.638	1.00	37.94
ATOM	1693	CE1	TYR	1701	30.977	4.955	8.535	1.00	40.79
ATOM	1694	CD2	TYR	1701	33.293	5.495	9.990	1.00	37.49
ATOM	1695	CE2	TYR	1701	33.351	4.646	8.886	1.00	41.82
ATOM	1696	CZ	TYR	1701	32.190	4.382	8.160	1.00	45.96
ATOM	1697	OH	TYR	1701	32.251	3.572	7.039	1.00	55.61
ATOM	1698	C	TYR	1701	32.377	7.559	13.970	1.00	32.85
ATOM	1699	O	TYR	1701	32.066	8.711	13.679	1.00	32.41
ATOM	1700	N	PRO	1702	32.753	7.229	15.215	1.00	34.48
ATOM	1701	CD	PRO	1702	33.288	5.946	15.695	1.00	35.64
ATOM	1702	CA	PRO	1702	32.775	8.258	16.270	1.00	33.68
ATOM	1703	CB	PRO	1702	33.321	7.499	17.482	1.00	32.52
ATOM	1704	CG	PRO	1702	33.063	6.061	17.166	1.00	38.81
ATOM	1705	C	PRO	1702	33.736	9.388	15.919	1.00	33.47
ATOM	1706	O	PRO	1702	34.875	9.145	15.522	1.00	34.66
ATOM	1707	N	GLY	1703	33.275	10.625	16.089	1.00	35.31
ATOM	1708	CA	GLY	1703	34.101	11.792	15.802	1.00	32.51
ATOM	1709	C	GLY	1703	34.232	12.166	14.339	1.00	33.68
ATOM	1710	O	GLY	1703	34.904	13.146	14.005	1.00	31.22

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ATOM	1711	N	VAL	1704	33.583	11.404	13.462	1.00	35.00
ATOM	1712	CA	VAL	1704	33.641	11.658	12.026	1.00	33.25
ATOM	1713	CB	VAL	1704	33.679	10.335	11.241	1.00	31.04
ATOM	1714	CG1	VAL	1704	33.825	10.605	9.766	1.00	32.72
ATOM	1715	CG2	VAL	1704	34.825	9.477	11.727	1.00	26.97
ATOM	1716	C	VAL	1704	32.475	12.529	11.533	1.00	34.75
ATOM	1717	O	VAL	1704	31.316	12.151	11.643	1.00	36.79
ATOM	1718	N	PRO	1705	32.787	13.735	11.032	1.00	35.01
ATOM	1719	CD	PRO	1705	34.133	14.333	11.086	1.00	35.61
ATOM	1720	CA	PRO	1705	31.801	14.685	10.512	1.00	35.33
ATOM	1721	CB	PRO	1705	32.539	16.020	10.617	1.00	35.59
ATOM	1722	CG	PRO	1705	33.950	15.625	10.339	1.00	37.23
ATOM	1723	C	PRO	1705	31.388	14.375	9.074	1.00	36.33
ATOM	1724	O	PRO	1705	32.125	13.695	8.355	1.00	38.44
ATOM	1725	N	VAL	1706	30.240	14.912	8.649	1.00	34.93
ATOM	1726	CA	VAL	1706	29.675	14.704	7.303	1.00	35.19
ATOM	1727	CB	VAL	1706	28.607	15.791	6.984	1.00	36.19
ATOM	1728	CG1	VAL	1706	28.011	15.586	5.586	1.00	36.30
ATOM	1729	CG2	VAL	1706	27.494	15.739	8.028	1.00	32.74
ATOM	1730	C	VAL	1706	30.696	14.632	6.155	1.00	36.20
ATOM	1731	O	VAL	1706	30.796	13.618	5.463	1.00	38.16
ATOM	1732	N	GLU	1707	31.479	15.695	6.020	1.00	34.38
ATOM	1733	CA	GLU	1707	32.500	15.819	4.987	1.00	33.75
ATOM	1734	CB	GLU	1707	33.181	17.184	5.083	1.00	35.79
ATOM	1735	C	GLU	1707	33.567	14.731	4.982	1.00	31.97
ATOM	1736	O	GLU	1707	34.036	14.311	3.923	1.00	32.84
ATOM	1737	N	GLU	1708	33.964	14.280	6.160	1.00	29.57
ATOM	1738	CA	GLU	1708	34.987	13.249	6.249	1.00	31.32
ATOM	1739	CB	GLU	1708	35.567	13.204	7.664	1.00	36.11
ATOM	1740	CG	GLU	1708	36.189	14.508	8.144	1.00	44.10
ATOM	1741	CD	GLU	1708	37.444	14.923	7.383	1.00	55.58
ATOM	1742	OE1	GLU	1708	38.059	14.082	6.681	1.00	61.47
ATOM	1743	OE2	GLU	1708	37.830	16.115	7.517	1.00	60.54
ATOM	1744	C	GLU	1708	34.365	11.906	5.889	1.00	32.20
ATOM	1745	O	GLU	1708	35.013	11.041	5.294	1.00	32.39
ATOM	1746	N	LEU	1709	33.094	11.749	6.245	1.00	31.43
ATOM	1747	CA	LEU	1709	32.378	10.522	5.961	1.00	31.71
ATOM	1748	CB	LEU	1709	30.973	10.548	6.565	1.00	28.84
ATOM	1749	CG	LEU	1709	30.136	9.357	6.081	1.00	28.28
ATOM	1750	CD1	LEU	1709	30.662	8.059	6.679	1.00	27.34
ATOM	1751	CD2	LEU	1709	28.705	9.556	6.437	1.00	29.71
ATOM	1752	C	LEU	1709	32.306	10.317	4.454	1.00	30.55
ATOM	1753	O	LEU	1709	32.489	9.202	3.970	1.00	31.79
ATOM	1754	N	PHE	1710	32.043	11.399	3.727	1.00	30.99
ATOM	1755	CA	PHE	1710	31.945	11.366	2.279	1.00	32.80
ATOM	1756	CB	PHE	1710	31.680	12.768	1.737	1.00	34.22
ATOM	1757	CG	PHE	1710	30.310	13.261	2.020	1.00	37.65
ATOM	1758	CD1	PHE	1710	29.337	12.393	2.495	1.00	43.43
ATOM	1759	CD2	PHE	1710	29.984	14.596	1.838	1.00	42.87
ATOM	1760	CE1	PHE	1710	28.054	12.834	2.787	1.00	46.00
ATOM	1761	CE2	PHE	1710	28.698	15.053	2.130	1.00	46.30
ATOM	1762	CZ	PHE	1710	27.733	14.169	2.605	1.00	46.49

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ATOM	1763	C	PHE	1710	33.196	10.802	1.667	1.00	34.25
ATOM	1764	O	PHE	1710	33.133	9.948	0.785	1.00	36.09
ATOM	1765	N	LYS	1711	34.324	11.249	2.209	1.00	34.37
ATOM	1766	CA	LYS	1711	35.664	10.840	1.789	1.00	34.11
ATOM	1767	CB	LYS	1711	36.672	11.768	2.476	1.00	37.74
ATOM	1768	CG	LYS	1711	38.114	11.567	2.119	1.00	43.59
ATOM	1769	CD	LYS	1711	38.978	12.573	2.857	1.00	46.97
ATOM	1770	CE	LYS	1711	40.386	12.575	2.304	1.00	51.53
ATOM	1771	NZ	LYS	1711	41.074	11.291	2.603	1.00	58.84
ATOM	1772	C	LYS	1711	35.948	9.354	2.103	1.00	33.25
ATOM	1773	O	LYS	1711	36.512	8.641	1.274	1.00	32.22
ATOM	1774	N	LEU	1712	35.537	8.894	3.285	1.00	32.62
ATOM	1775	CA	LEU	1712	35.718	7.496	3.667	1.00	31.41
ATOM	1776	CB	LEU	1712	35.223	7.237	5.106	1.00	29.80
ATOM	1777	CG	LEU	1712	36.020	7.889	6.244	1.00	29.22
ATOM	1778	CD1	LEU	1712	35.385	7.643	7.608	1.00	24.09
ATOM	1779	CD2	LEU	1712	37.437	7.356	6.234	1.00	28.36
ATOM	1780	C	LEU	1712	34.939	6.638	2.674	1.00	31.88
ATOM	1781	O	LEU	1712	35.452	5.654	2.143	1.00	34.08
ATOM	1782	N	LEU	1713	33.700	7.029	2.413	1.00	32.28
ATOM	1783	CA	LEU	1713	32.850	6.305	1.482	1.00	35.36
ATOM	1784	CB	LEU	1713	31.433	6.887	1.485	1.00	38.97
ATOM	1785	CG	LEU	1713	30.629	6.494	2.730	1.00	39.56
ATOM	1786	CD1	LEU	1713	29.308	7.228	2.768	1.00	37.14
ATOM	1787	CD2	LEU	1713	30.424	4.988	2.748	1.00	37.73
ATOM	1788	C	LEU	1713	33.430	6.296	0.070	1.00	36.47
ATOM	1789	O	LEU	1713	33.502	5.244	-0.563	1.00	39.32
ATOM	1790	N	LYS	1714	33.855	7.455	-0.413	1.00	35.21
ATOM	1791	CA	LYS	1714	34.437	7.544	-1.743	1.00	34.55
ATOM	1792	CB	LYS	1714	34.812	8.984	-2.075	1.00	34.81
ATOM	1793	CG	LYS	1714	33.624	9.903	-2.290	1.00	36.55
ATOM	1794	CD	LYS	1714	32.681	9.372	-3.353	1.00	40.68
ATOM	1795	CE	LYS	1714	31.488	10.310	-3.577	1.00	44.87
ATOM	1796	NZ	LYS	1714	30.611	9.853	-4.701	1.00	50.99
ATOM	1797	C	LYS	1714	35.671	6.649	-1.856	1.00	35.97
ATOM	1798	O	LYS	1714	35.948	6.084	-2.920	1.00	38.11
ATOM	1799	N	GLU	1715	36.385	6.490	-0.749	1.00	33.65
ATOM	1800	CA	GLU	1715	37.582	5.663	-0.729	1.00	34.34
ATOM	1801	CB	GLU	1715	38.574	6.221	0.288	1.00	34.90
ATOM	1802	CG	GLU	1715	39.032	7.613	-0.110	1.00	42.07
ATOM	1803	CD	GLU	1715	39.729	8.405	0.989	1.00	47.94
ATOM	1804	OE1	GLU	1715	39.977	7.870	2.098	1.00	45.03
ATOM	1805	OE2	GLU	1715	40.026	9.596	0.709	1.00	51.48
ATOM	1806	C	GLU	1715	37.285	4.191	-0.466	1.00	34.76
ATOM	1807	O	GLU	1715	38.205	3.384	-0.411	1.00	37.36
ATOM	1808	N	GLY	1716	36.002	3.848	-0.347	1.00	32.00
ATOM	1809	CA	GLY	1716	35.604	2.474	-0.122	1.00	30.49
ATOM	1810	C	GLY	1716	35.932	1.937	1.251	1.00	31.32
ATOM	1811	O	GLY	1716	36.134	0.738	1.430	1.00	31.83
ATOM	1812	N	HIS	1717	35.957	2.822	2.233	1.00	31.55
ATOM	1813	CA	HIS	1717	36.265	2.416	3.595	1.00	33.20
ATOM	1814	CB	HIS	1717	36.494	3.661	4.452	1.00	37.67

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ATOM	1815	CG	HIS	1717	36.786	3.360	5.895	1.00	42.42
ATOM	1816	CD2	HIS	1717	37.957	3.259	6.567	1.00	40.97
ATOM	1817	ND1	HIS	1717	35.789	3.142	6.825	1.00	45.02
ATOM	1818	CE1	HIS	1717	36.333	2.914	8.004	1.00	44.06
ATOM	1819	NE2	HIS	1717	37.645	2.976	7.873	1.00	43.67
ATOM	1820	C	HIS	1717	35.149	1.567	4.201	1.00	31.72
ATOM	1821	O	HIS	1717	33.975	1.816	3.952	1.00	32.12
ATOM	1822	N	ARG	1718	35.529	0.582	5.009	1.00	31.09
ATOM	1823	CA	ARG	1718	34.586	-0.288	5.696	1.00	32.10
ATOM	1824	CB	ARG	1718	34.531	-1.664	5.024	1.00	31.61
ATOM	1825	CG	ARG	1718	34.048	-1.651	3.577	1.00	31.32
ATOM	1826	CD	ARG	1718	32.579	-1.263	3.495	1.00	29.60
ATOM	1827	NE	ARG	1718	32.036	-1.320	2.129	1.00	24.72
ATOM	1828	CZ	ARG	1718	32.103	-0.324	1.243	1.00	22.01
ATOM	1829	NH1	ARG	1718	32.709	0.819	1.554	1.00	19.00
ATOM	1830	NH2	ARG	1718	31.463	-0.444	0.083	1.00	14.18
ATOM	1831	C	ARG	1718	35.042	-0.438	7.164	1.00	33.81
ATOM	1832	O	ARG	1718	36.234	-0.596	7.446	1.00	34.62
ATOM	1833	N	MET	1719	34.084	-0.372	8.085	1.00	33.99
ATOM	1834	CA	MET	1719	34.382	-0.466	9.508	1.00	32.51
ATOM	1835	CB	MET	1719	33.110	-0.246	10.342	1.00	33.51
ATOM	1836	CG	MET	1719	32.513	1.155	10.200	1.00	33.69
ATOM	1837	SD	MET	1719	31.082	1.526	11.251	1.00	37.49
ATOM	1838	CE	MET	1719	29.906	0.373	10.618	1.00	37.62
ATOM	1839	C	MET	1719	35.033	-1.799	9.844	1.00	32.92
ATOM	1840	O	MET	1719	34.900	-2.772	9.098	1.00	33.67
ATOM	1841	N	ASP	1720	35.776	-1.825	10.945	1.00	35.49
ATOM	1842	CA	ASP	1720	36.466	-3.038	11.388	1.00	36.87
ATOM	1843	CB	ASP	1720	37.585	-2.694	12.376	1.00	41.64
ATOM	1844	CG	ASP	1720	38.688	-1.859	11.754	1.00	46.44
ATOM	1845	OD1	ASP	1720	38.507	-1.410	10.604	1.00	52.86
ATOM	1846	OD2	ASP	1720	39.740	-1.650	12.422	1.00	46.76
ATOM	1847	C	ASP	1720	35.516	-4.005	12.053	1.00	34.70
ATOM	1848	O	ASP	1720	34.459	-3.603	12.548	1.00	34.31
ATOM	1849	N	LYS	1721	35.937	-5.265	12.132	1.00	33.39
ATOM	1850	CA	LYS	1721	35.119	-6.297	12.755	1.00	32.68
ATOM	1851	CB	LYS	1721	35.692	-7.690	12.500	1.00	33.55
ATOM	1852	CG	LYS	1721	34.834	-8.791	13.119	1.00	33.62
ATOM	1853	CD	LYS	1721	35.336	-10.158	12.771	1.00	35.77
ATOM	1854	CE	LYS	1721	36.082	-10.747	13.931	1.00	38.73
ATOM	1855	NZ	LYS	1721	36.325	-12.190	13.711	1.00	43.86
ATOM	1856	C	LYS	1721	35.034	-6.107	14.240	1.00	34.61
ATOM	1857	O	LYS	1721	36.057	-5.944	14.905	1.00	37.05
ATOM	1858	N	PRO	1722	33.808	-6.092	14.781	1.00	36.16
ATOM	1859	CD	PRO	1722	32.518	-6.062	14.066	1.00	34.73
ATOM	1860	CA	PRO	1722	33.611	-5.926	16.222	1.00	37.84
ATOM	1861	CB	PRO	1722	32.095	-6.017	16.360	1.00	37.19
ATOM	1862	CG	PRO	1722	31.607	-5.448	15.073	1.00	36.00
ATOM	1863	C	PRO	1722	34.266	-7.109	16.950	1.00	39.95
ATOM	1864	O	PRO	1722	34.340	-8.218	16.406	1.00	38.82
ATOM	1865	N	SER	1723	34.783	-6.884	18.150	1.00	42.36
ATOM	1866	CA	SER	1723	35.359	-7.995	18.890	1.00	45.70

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ATOM	1867	CB	SER	1723	36.170	-7.511	20.093	1.00	47.50
ATOM	1868	OG	SER	1723	35.341	-6.964	21.100	1.00	55.28
ATOM	1869	C	SER	1723	34.136	-8.784	19.346	1.00	46.70
ATOM	1870	O	SER	1723	33.037	-8.224	19.477	1.00	47.27
ATOM	1871	N	ASN	1724	34.296	-10.081	19.559	1.00	47.84
ATOM	1872	CA	ASN	1724	33.174	-10.900	19.992	1.00	51.26
ATOM	1873	CB	ASN	1724	32.620	-10.361	21.330	1.00	57.15
ATOM	1874	CG	ASN	1724	33.732	-10.088	22.365	1.00	61.53
ATOM	1875	OD1	ASN	1724	34.565	-10.955	22.646	1.00	64.13
ATOM	1876	ND2	ASN	1724	33.763	-8.867	22.912	1.00	61.69
ATOM	1877	C	ASN	1724	32.101	-10.916	18.873	1.00	50.72
ATOM	1878	O	ASN	1724	30.925	-10.617	19.089	1.00	52.63
ATOM	1879	N	CYS	1725	32.564	-11.193	17.663	1.00	48.01
ATOM	1880	CA	CYS	1725	31.719	-11.295	16.478	1.00	45.16
ATOM	1881	CB	CYS	1725	31.603	-9.929	15.788	1.00	44.77
ATOM	1882	SG	CYS	1725	30.605	-9.929	14.272	1.00	40.74
ATOM	1883	C	CYS	1725	32.421	-12.308	15.570	1.00	41.51
ATOM	1884	O	CYS	1725	33.639	-12.236	15.397	1.00	42.47
ATOM	1885	N	THR	1726	31.677	-13.289	15.064	1.00	37.54
ATOM	1886	CA	THR	1726	32.268	-14.313	14.202	1.00	35.03
ATOM	1887	CB	THR	1726	31.308	-15.500	13.993	1.00	31.87
ATOM	1888	OG1	THR	1726	30.074	-15.042	13.406	1.00	32.84
ATOM	1889	CG2	THR	1726	31.017	-16.160	15.306	1.00	29.78
ATOM	1890	C	THR	1726	32.678	-13.770	12.845	1.00	34.76
ATOM	1891	O	THR	1726	32.180	-12.729	12.415	1.00	38.22
ATOM	1892	N	ASN	1727	33.596	-14.450	12.175	1.00	32.47
ATOM	1893	CA	ASN	1727	34.009	-14.024	10.842	1.00	34.75
ATOM	1894	CB	ASN	1727	35.167	-14.872	10.308	1.00	39.77
ATOM	1895	CG	ASN	1727	36.464	-14.591	11.026	1.00	46.09
ATOM	1896	OD1	ASN	1727	37.019	-13.495	10.933	1.00	49.54
ATOM	1897	ND2	ASN	1727	36.961	-15.585	11.749	1.00	50.04
ATOM	1898	C	ASN	1727	32.825	-14.147	9.905	1.00	33.38
ATOM	1899	O	ASN	1727	32.726	-13.405	8.929	1.00	34.10
ATOM	1900	N	GLU	1728	31.916	-15.065	10.224	1.00	32.01
ATOM	1901	CA	GLU	1728	30.707	-15.310	9.418	1.00	30.41
ATOM	1902	CB	GLU	1728	30.010	-16.580	9.917	1.00	32.27
ATOM	1903	CG	GLU	1728	28.811	-17.034	9.094	1.00	31.55
ATOM	1904	CD	GLU	1728	28.251	-18.369	9.577	1.00	36.38
ATOM	1905	OE1	GLU	1728	28.415	-18.694	10.777	1.00	38.35
ATOM	1906	OE2	GLU	1728	27.632	-19.086	8.758	1.00	36.34
ATOM	1907	C	GLU	1728	29.749	-14.119	9.468	1.00	29.40
ATOM	1908	O	GLU	1728	29.231	-13.679	8.438	1.00	26.23
ATOM	1909	N	LEU	1729	29.520	-13.610	10.672	1.00	29.19
ATOM	1910	CA	LEU	1729	28.645	-12.462	10.849	1.00	30.26
ATOM	1911	CB	LEU	1729	28.215	-12.343	12.310	1.00	30.74
ATOM	1912	CG	LEU	1729	27.198	-13.410	12.721	1.00	31.27
ATOM	1913	CD1	LEU	1729	27.013	-13.377	14.226	1.00	33.65
ATOM	1914	CD2	LEU	1729	25.865	-13.161	12.010	1.00	26.16
ATOM	1915	C	LEU	1729	29.269	-11.161	10.335	1.00	28.79
ATOM	1916	O	LEU	1729	28.548	-10.255	9.914	1.00	30.60
ATOM	1917	N	TYR	1730	30.594	-11.069	10.363	1.00	26.64
ATOM	1918	CA	TYR	1730	31.281	-9.881	9.844	1.00	26.47

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ATOM	1919	CB	TYR	1730	32.742	-9.869	10.298	1.00	24.31
ATOM	1920	CG	TYR	1730	33.512	-8.670	9.805	1.00	25.61
ATOM	1921	CD1	TYR	1730	33.029	-7.373	10.016	1.00	25.68
ATOM	1922	CE1	TYR	1730	33.691	-6.264	9.496	1.00	23.70
ATOM	1923	CD2	TYR	1730	34.688	-8.826	9.067	1.00	24.48
ATOM	1924	CE2	TYR	1730	35.361	-7.719	8.537	1.00	22.61
ATOM	1925	CZ	TYR	1730	34.856	-6.445	8.748	1.00	24.41
ATOM	1926	OH	TYR	1730	35.476	-5.354	8.176	1.00	24.37
ATOM	1927	C	TYR	1730	31.186	-9.902	8.301	1.00	26.06
ATOM	1928	O	TYR	1730	30.981	-8.881	7.651	1.00	23.68
ATOM	1929	N	MET	1731	31.347	-11.084	7.727	1.00	26.60
ATOM	1930	CA	MET	1731	31.247	-11.270	6.299	1.00	29.90
ATOM	1931	CB	MET	1731	31.475	-12.740	5.968	1.00	38.39
ATOM	1932	CG	MET	1731	31.076	-13.157	4.577	1.00	52.98
ATOM	1933	SD	MET	1731	31.612	-14.831	4.216	1.00	69.59
ATOM	1934	CE	MET	1731	32.659	-14.506	2.727	1.00	66.05
ATOM	1935	C	MET	1731	29.864	-10.819	5.840	1.00	29.05
ATOM	1936	O	MET	1731	29.720	-10.194	4.791	1.00	30.94
ATOM	1937	N	MET	1732	28.845	-11.134	6.633	1.00	29.40
ATOM	1938	CA	MET	1732	27.475	-10.743	6.328	1.00	26.97
ATOM	1939	CB	MET	1732	26.537	-11.293	7.398	1.00	25.73
ATOM	1940	CG	MET	1732	25.068	-10.984	7.156	1.00	26.01
ATOM	1941	SD	MET	1732	23.980	-11.637	8.407	1.00	26.97
ATOM	1942	CE	MET	1732	23.773	-13.354	7.798	1.00	21.23
ATOM	1943	C	MET	1732	27.387	-9.220	6.271	1.00	27.49
ATOM	1944	O	MET	1732	26.778	-8.661	5.361	1.00	29.17
ATOM	1945	N	MET	1733	27.982	-8.550	7.259	1.00	27.79
ATOM	1946	CA	MET	1733	28.001	-7.090	7.293	1.00	27.41
ATOM	1947	CB	MET	1733	28.797	-6.587	8.484	1.00	28.84
ATOM	1948	CG	MET	1733	28.153	-6.761	9.829	1.00	32.18
ATOM	1949	SD	MET	1733	29.300	-6.248	11.127	1.00	32.77
ATOM	1950	CE	MET	1733	28.850	-7.423	12.399	1.00	33.03
ATOM	1951	C	MET	1733	28.711	-6.599	6.035	1.00	28.54
ATOM	1952	O	MET	1733	28.250	-5.680	5.357	1.00	30.69
ATOM	1953	N	ARG	1734	29.865	-7.194	5.751	1.00	28.59
ATOM	1954	CA	ARG	1734	30.650	-6.831	4.571	1.00	29.53
ATOM	1955	CB	ARG	1734	31.970	-7.609	4.531	1.00	28.74
ATOM	1956	CG	ARG	1734	32.944	-7.245	5.638	1.00	26.75
ATOM	1957	CD	ARG	1734	33.158	-5.755	5.702	1.00	26.58
ATOM	1958	NE	ARG	1734	33.825	-5.288	4.499	1.00	34.72
ATOM	1959	CZ	ARG	1734	35.139	-5.360	4.306	1.00	37.67
ATOM	1960	NH1	ARG	1734	35.927	-5.867	5.251	1.00	40.46
ATOM	1961	NH2	ARG	1734	35.663	-4.986	3.147	1.00	38.11
ATOM	1962	C	ARG	1734	29.855	-7.051	3.294	1.00	28.03
ATOM	1963	O	ARG	1734	29.958	-6.260	2.359	1.00	27.22
ATOM	1964	N	ASP	1735	29.071	-8.130	3.260	1.00	27.81
ATOM	1965	CA	ASP	1735	28.212	-8.436	2.103	1.00	27.27
ATOM	1966	CB	ASP	1735	27.608	-9.835	2.216	1.00	28.62
ATOM	1967	CG	ASP	1735	28.638	-10.932	2.075	1.00	30.15
ATOM	1968	OD1	ASP	1735	29.745	-10.663	1.553	1.00	31.23
ATOM	1969	OD2	ASP	1735	28.354	-12.070	2.501	1.00	32.00
ATOM	1970	C	ASP	1735	27.099	-7.400	1.971	1.00	24.78

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ATOM	1971	O	ASP	1735	26.714	-7.068	0.852	1.00	24.52
ATOM	1972	N	CYS	1736	26.590	-6.908	3.104	1.00	24.10
ATOM	1973	CA	CYS	1736	25.530	-5.871	3.140	1.00	25.20
ATOM	1974	CB	CYS	1736	24.965	-5.679	4.569	1.00	23.85
ATOM	1975	SG	CYS	1736	23.898	-7.030	5.143	1.00	18.77
ATOM	1976	C	CYS	1736	26.042	-4.520	2.611	1.00	23.39
ATOM	1977	O	CYS	1736	25.276	-3.718	2.070	1.00	21.76
ATOM	1978	N	TRP	1737	27.348	-4.303	2.743	1.00	23.53
ATOM	1979	CA	TRP	1737	27.988	-3.072	2.302	1.00	21.57
ATOM	1980	CB	TRP	1737	29.026	-2.631	3.314	1.00	18.82
ATOM	1981	CG	TRP	1737	28.485	-2.418	4.686	1.00	19.89
ATOM	1982	CD2	TRP	1737	29.194	-2.609	5.913	1.00	22.39
ATOM	1983	CE2	TRP	1737	28.329	-2.213	6.959	1.00	21.78
ATOM	1984	CE3	TRP	1737	30.478	-3.083	6.238	1.00	23.52
ATOM	1985	CD1	TRP	1737	27.248	-1.932	5.022	1.00	19.40
ATOM	1986	NE1	TRP	1737	27.147	-1.805	6.383	1.00	21.52
ATOM	1987	CZ2	TRP	1737	28.705	-2.270	8.319	1.00	21.85
ATOM	1988	CZ3	TRP	1737	30.857	-3.134	7.583	1.00	25.30
ATOM	1989	CH2	TRP	1737	29.972	-2.728	8.604	1.00	26.17
ATOM	1990	C	TRP	1737	28.673	-3.226	0.956	1.00	24.49
ATOM	1991	O	TRP	1737	29.648	-2.519	0.670	1.00	25.09
ATOM	1992	N	HIS	1738	28.203	-4.170	0.136	1.00	25.12
ATOM	1993	CA	HIS	1738	28.808	-4.341	-1.172	1.00	22.90
ATOM	1994	CB	HIS	1738	28.163	-5.497	-1.928	1.00	23.14
ATOM	1995	CG	HIS	1738	29.017	-6.013	-3.051	1.00	23.26
ATOM	1996	CD2	HIS	1738	29.550	-5.380	-4.129	1.00	23.78
ATOM	1997	ND1	HIS	1738	29.492	-7.308	-3.104	1.00	24.91
ATOM	1998	CE1	HIS	1738	30.286	-7.445	-4.156	1.00	25.29
ATOM	1999	NE2	HIS	1738	30.341	-6.288	-4.794	1.00	26.99
ATOM	2000	C	HIS	1738	28.670	-3.024	-1.958	1.00	22.92
ATOM	2001	O	HIS	1738	27.615	-2.381	-1.933	1.00	20.27
ATOM	2002	N	ALA	1739	29.752	-2.608	-2.607	1.00	24.30
ATOM	2003	CA	ALA	1739	29.762	-1.378	-3.385	1.00	23.70
ATOM	2004	CB	ALA	1739	31.079	-1.234	-4.076	1.00	25.24
ATOM	2005	C	ALA	1739	28.645	-1.391	-4.416	1.00	25.37
ATOM	2006	O	ALA	1739	27.955	-0.391	-4.606	1.00	27.86
ATOM	2007	N	VAL	1740	28.507	-2.521	-5.102	1.00	23.97
ATOM	2008	CA	VAL	1740	27.481	-2.700	-6.121	1.00	24.64
ATOM	2009	CB	VAL	1740	27.966	-3.698	-7.206	1.00	26.39
ATOM	2010	CG1	VAL	1740	27.013	-3.757	-8.360	1.00	22.65
ATOM	2011	CG2	VAL	1740	29.308	-3.260	-7.720	1.00	27.43
ATOM	2012	C	VAL	1740	26.170	-3.209	-5.481	1.00	23.97
ATOM	2013	O	VAL	1740	26.126	-4.347	-4.978	1.00	24.14
ATOM	2014	N	PRO	1741	25.090	-2.397	-5.545	1.00	22.77
ATOM	2015	CD	PRO	1741	25.074	-1.093	-6.237	1.00	17.82
ATOM	2016	CA	PRO	1741	23.763	-2.695	-4.980	1.00	23.22
ATOM	2017	CB	PRO	1741	22.891	-1.554	-5.526	1.00	18.19
ATOM	2018	CG	PRO	1741	23.866	-0.419	-5.647	1.00	15.09
ATOM	2019	C	PRO	1741	23.189	-4.074	-5.343	1.00	23.26
ATOM	2020	O	PRO	1741	22.700	-4.788	-4.462	1.00	22.42
ATOM	2021	N	SER	1742	23.335	-4.473	-6.615	1.00	23.49
ATOM	2022	CA	SER	1742	22.826	-5.754	-7.119	1.00	23.17

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ATOM	2023	CB	SER	1742	22.956	-5.808	-8.641	1.00	23.67
ATOM	2024	OG	SER	1742	24.324	-5.891	-9.023	1.00	26.64
ATOM	2025	C	SER	1742	23.524	-6.984	-6.545	1.00	23.09
ATOM	2026	O	SER	1742	22.993	-8.104	-6.603	1.00	21.90
ATOM	2027	N	GLN	1743	24.719	-6.782	-5.997	1.00	23.62
ATOM	2028	CA	GLN	1743	25.466	-7.895	-5.416	1.00	23.26
ATOM	2029	CB	GLN	1743	26.953	-7.754	-5.702	1.00	24.32
ATOM	2030	CG	GLN	1743	27.255	-7.828	-7.170	1.00	23.04
ATOM	2031	CD	GLN	1743	26.684	-9.076	-7.810	1.00	24.83
ATOM	2032	OE1	GLN	1743	27.176	-10.178	-7.584	1.00	21.07
ATOM	2033	NE2	GLN	1743	25.647	-8.907	-8.625	1.00	22.66
ATOM	2034	C	GLN	1743	25.227	-8.121	-3.927	1.00	23.85
ATOM	2035	O	GLN	1743	25.744	-9.083	-3.366	1.00	25.36
ATOM	2036	N	ARG	1744	24.458	-7.240	-3.290	1.00	22.69
ATOM	2037	CA	ARG	1744	24.155	-7.395	-1.868	1.00	21.65
ATOM	2038	CB	ARG	1744	23.635	-6.087	-1.277	1.00	21.22
ATOM	2039	CG	ARG	1744	24.623	-4.962	-1.342	1.00	21.63
ATOM	2040	CD	ARG	1744	24.013	-3.656	-0.863	1.00	19.06
ATOM	2041	NE	ARG	1744	24.869	-2.563	-1.318	1.00	24.44
ATOM	2042	CZ	ARG	1744	24.461	-1.322	-1.564	1.00	22.49
ATOM	2043	NH1	ARG	1744	23.184	-0.972	-1.378	1.00	18.95
ATOM	2044	NH2	ARG	1744	25.337	-0.438	-2.034	1.00	22.19
ATOM	2045	C	ARG	1744	23.095	-8.470	-1.712	1.00	22.45
ATOM	2046	O	ARG	1744	22.363	-8.772	-2.654	1.00	25.62
ATOM	2047	N	PRO	1745	23.065	-9.139	-0.559	1.00	21.78
ATOM	2048	CD	PRO	1745	24.025	-9.114	0.563	1.00	21.02
ATOM	2049	CA	PRO	1745	22.057	-10.175	-0.362	1.00	20.99
ATOM	2050	CB	PRO	1745	22.532	-10.879	0.919	1.00	21.12
ATOM	2051	CG	PRO	1745	23.240	-9.777	1.676	1.00	19.86
ATOM	2052	C	PRO	1745	20.726	-9.485	-0.146	1.00	22.18
ATOM	2053	O	PRO	1745	20.680	-8.281	0.128	1.00	23.04
ATOM	2054	N	THR	1746	19.646	-10.236	-0.297	1.00	19.31
ATOM	2055	CA	THR	1746	18.335	-9.689	-0.085	1.00	19.12
ATOM	2056	CB	THR	1746	17.307	-10.334	-1.045	1.00	19.86
ATOM	2057	OG1	THR	1746	17.299	-11.763	-0.886	1.00	22.54
ATOM	2058	CG2	THR	1746	17.668	-10.002	-2.479	1.00	22.97
ATOM	2059	C	THR	1746	17.961	-9.975	1.367	1.00	19.91
ATOM	2060	O	THR	1746	18.676	-10.711	2.058	1.00	19.93
ATOM	2061	N	PHE	1747	16.884	-9.381	1.855	1.00	21.80
ATOM	2062	CA	PHE	1747	16.456	-9.678	3.224	1.00	23.46
ATOM	2063	CB	PHE	1747	15.353	-8.720	3.686	1.00	21.84
ATOM	2064	CG	PHE	1747	15.872	-7.368	4.082	1.00	24.84
ATOM	2065	CD1	PHE	1747	16.627	-7.207	5.237	1.00	22.23
ATOM	2066	CD2	PHE	1747	15.611	-6.248	3.293	1.00	22.97
ATOM	2067	CE1	PHE	1747	17.124	-5.944	5.598	1.00	19.42
ATOM	2068	CE2	PHE	1747	16.111	-4.991	3.646	1.00	17.14
ATOM	2069	CZ	PHE	1747	16.862	-4.846	4.801	1.00	18.02
ATOM	2070	C	PHE	1747	15.992	-11.133	3.295	1.00	22.28
ATOM	2071	O	PHE	1747	16.189	-11.796	4.304	1.00	23.76
ATOM	2072	N	LYS	1748	15.430	-11.632	2.199	1.00	23.46
ATOM	2073	CA	LYS	1748	14.971	-13.014	2.140	1.00	25.84
ATOM	2074	CB	LYS	1748	14.344	-13.327	0.782	1.00	26.89

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ATOM	2075	CG	LYS	1748	14.061	-14.793	0.583	1.00	31.07
ATOM	2076	CD	LYS	1748	13.714	-15.064	-0.861	1.00	37.82
ATOM	2077	CE	LYS	1748	13.231	-16.493	-1.068	1.00	44.36
ATOM	2078	NZ	LYS	1748	12.027	-16.782	-0.235	1.00	50.16
ATOM	2079	C	LYS	1748	16.160	-13.949	2.393	1.00	27.27
ATOM	2080	O	LYS	1748	16.067	-14.877	3.202	1.00	27.87
ATOM	2081	N	GLN	1749	17.288	-13.674	1.730	1.00	25.64
ATOM	2082	CA	GLN	1749	18.507	-14.457	1.903	1.00	24.32
ATOM	2083	CB	GLN	1749	19.608	-13.938	0.983	1.00	28.87
ATOM	2084	CG	GLN	1749	19.343	-14.049	-0.496	1.00	36.24
ATOM	2085	CD	GLN	1749	20.437	-13.374	-1.318	1.00	41.30
ATOM	2086	OE1	GLN	1749	20.173	-12.422	-2.044	1.00	38.35
ATOM	2087	NE2	GLN	1749	21.683	-13.861	-1.190	1.00	45.38
ATOM	2088	C	GLN	1749	19.002	-14.310	3.346	1.00	22.89
ATOM	2089	O	GLN	1749	19.302	-15.305	4.008	1.00	22.55
ATOM	2090	N	LEU	1750	19.114	-13.064	3.813	1.00	20.89
ATOM	2091	CA	LEU	1750	19.570	-12.776	5.167	1.00	21.44
ATOM	2092	CB	LEU	1750	19.471	-11.282	5.462	1.00	19.53
ATOM	2093	CG	LEU	1750	20.432	-10.400	4.663	1.00	19.14
ATOM	2094	CD1	LEU	1750	20.069	-8.919	4.816	1.00	14.53
ATOM	2095	CD2	LEU	1750	21.863	-10.685	5.106	1.00	16.18
ATOM	2096	C	LEU	1750	18.776	-13.538	6.208	1.00	22.98
ATOM	2097	O	LEU	1750	19.335	-14.057	7.183	1.00	23.12
ATOM	2098	N	VAL	1751	17.465	-13.586	6.020	1.00	23.48
ATOM	2099	CA	VAL	1751	16.610	-14.292	6.945	1.00	23.21
ATOM	2100	CB	VAL	1751	15.132	-14.075	6.590	1.00	20.94
ATOM	2101	CG1	VAL	1751	14.268	-15.008	7.375	1.00	21.67
ATOM	2102	CG2	VAL	1751	14.730	-12.649	6.929	1.00	20.32
ATOM	2103	C	VAL	1751	16.974	-15.774	6.990	1.00	26.13
ATOM	2104	O	VAL	1751	17.030	-16.379	8.058	1.00	26.35
ATOM	2105	N	GLU	1752	17.260	-16.348	5.831	1.00	30.05
ATOM	2106	CA	GLU	1752	17.632	-17.747	5.778	1.00	32.54
ATOM	2107	CB	GLU	1752	17.695	-18.221	4.338	1.00	38.54
ATOM	2108	CG	GLU	1752	16.322	-18.226	3.673	1.00	50.06
ATOM	2109	CD	GLU	1752	16.333	-18.759	2.247	1.00	56.55
ATOM	2110	OE1	GLU	1752	15.365	-18.480	1.507	1.00	61.63
ATOM	2111	OE2	GLU	1752	17.303	-19.466	1.875	1.00	59.57
ATOM	2112	C	GLU	1752	18.974	-17.965	6.486	1.00	31.62
ATOM	2113	O	GLU	1752	19.113	-18.858	7.322	1.00	29.63
ATOM	2114	N	ASP	1753	19.938	-17.103	6.193	1.00	30.74
ATOM	2115	CA	ASP	1753	21.246	-17.211	6.807	1.00	31.00
ATOM	2116	CB	ASP	1753	22.209	-16.181	6.203	1.00	31.47
ATOM	2117	CG	ASP	1753	22.445	-16.390	4.710	1.00	35.82
ATOM	2118	OD1	ASP	1753	22.396	-17.549	4.248	1.00	36.78
ATOM	2119	OD2	ASP	1753	22.671	-15.396	3.992	1.00	41.04
ATOM	2120	C	ASP	1753	21.158	-17.058	8.314	1.00	28.94
ATOM	2121	O	ASP	1753	21.597	-17.933	9.059	1.00	29.91
ATOM	2122	N	LEU	1754	20.526	-15.984	8.764	1.00	28.33
ATOM	2123	CA	LEU	1754	20.386	-15.731	10.199	1.00	26.88
ATOM	2124	CB	LEU	1754	19.724	-14.372	10.457	1.00	19.82
ATOM	2125	CG	LEU	1754	20.737	-13.269	10.154	1.00	20.90
ATOM	2126	CD1	LEU	1754	20.074	-11.886	9.995	1.00	14.83

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ATOM	2127	CD2	LEU	1754	21.831	-13.308	11.240	1.00	16.39
ATOM	2128	C	LEU	1754	19.645	-16.861	10.896	1.00	29.18
ATOM	2129	O	LEU	1754	20.030	-17.262	11.986	1.00	30.55
ATOM	2130	N	ASP	1755	18.638	-17.421	10.238	1.00	31.65
ATOM	2131	CA	ASP	1755	17.892	-18.517	10.822	1.00	31.78
ATOM	2132	CB	ASP	1755	16.723	-18.900	9.928	1.00	34.57
ATOM	2133	CG	ASP	1755	15.876	-19.997	10.533	1.00	38.29
ATOM	2134	OD1	ASP	1755	15.410	-19.844	11.677	1.00	45.68
ATOM	2135	OD2	ASP	1755	15.685	-21.031	9.878	1.00	43.09
ATOM	2136	C	ASP	1755	18.801	-19.713	11.034	1.00	33.50
ATOM	2137	O	ASP	1755	18.665	-20.428	12.025	1.00	34.39
ATOM	2138	N	ARG	1756	19.738	-19.907	10.107	1.00	35.51
ATOM	2139	CA	ARG	1756	20.700	-21.004	10.169	1.00	35.33
ATOM	2140	CB	ARG	1756	21.417	-21.125	8.825	1.00	38.41
ATOM	2141	CG	ARG	1756	22.522	-22.181	8.759	1.00	40.99
ATOM	2142	CD	ARG	1756	23.181	-22.223	7.376	1.00	44.60
ATOM	2143	NE	ARG	1756	23.676	-20.917	6.916	1.00	49.55
ATOM	2144	CZ	ARG	1756	24.795	-20.338	7.349	1.00	53.56
ATOM	2145	NH1	ARG	1756	25.556	-20.937	8.266	1.00	53.25
ATOM	2146	NH2	ARG	1756	25.165	-19.163	6.853	1.00	55.72
ATOM	2147	C	ARG	1756	21.719	-20.754	11.275	1.00	35.01
ATOM	2148	O	ARG	1756	22.000	-21.632	12.088	1.00	34.86
ATOM	2149	N	ILE	1757	22.244	-19.536	11.314	1.00	35.06
ATOM	2150	CA	ILE	1757	23.242	-19.153	12.302	1.00	35.25
ATOM	2151	CB	ILE	1757	23.847	-17.753	11.984	1.00	34.59
ATOM	2152	CG2	ILE	1757	24.915	-17.401	12.995	1.00	32.98
ATOM	2153	CG1	ILE	1757	24.481	-17.757	10.586	1.00	33.64
ATOM	2154	CD1	ILE	1757	24.812	-16.387	10.032	1.00	28.79
ATOM	2155	C	ILE	1757	22.673	-19.182	13.716	1.00	36.74
ATOM	2156	O	ILE	1757	23.283	-19.764	14.601	1.00	36.60
ATOM	2157	N	VAL	1758	21.489	-18.608	13.917	1.00	39.16
ATOM	2158	CA	VAL	1758	20.854	-18.589	15.243	1.00	41.06
ATOM	2159	CB	VAL	1758	19.378	-18.104	15.165	1.00	38.77
ATOM	2160	CG1	VAL	1758	18.715	-18.183	16.530	1.00	38.72
ATOM	2161	CG2	VAL	1758	19.309	-16.670	14.651	1.00	39.49
ATOM	2162	C	VAL	1758	20.885	-19.986	15.850	1.00	43.92
ATOM	2163	O	VAL	1758	21.403	-20.182	16.954	1.00	46.90
ATOM	2164	N	ALA	1759	20.370	-20.957	15.098	1.00	43.96
ATOM	2165	CA	ALA	1759	20.325	-22.354	15.528	1.00	43.47
ATOM	2166	CB	ALA	1759	19.653	-23.197	14.460	1.00	42.26
ATOM	2167	C	ALA	1759	21.693	-22.953	15.890	1.00	44.02
ATOM	2168	O	ALA	1759	21.780	-23.872	16.697	1.00	45.94
ATOM	2169	N	LEU	1760	22.750	-22.465	15.255	1.00	45.07
ATOM	2170	CA	LEU	1760	24.095	-22.949	15.514	1.00	46.72
ATOM	2171	CB	LEU	1760	24.899	-22.900	14.225	1.00	48.22
ATOM	2172	CG	LEU	1760	24.279	-23.645	13.053	1.00	51.98
ATOM	2173	CD1	LEU	1760	25.016	-23.279	11.778	1.00	56.19
ATOM	2174	CD2	LEU	1760	24.327	-25.136	13.313	1.00	52.82
ATOM	2175	C	LEU	1760	24.811	-22.118	16.578	1.00	47.59
ATOM	2176	O	LEU	1760	25.935	-22.432	16.986	1.00	44.63
ATOM	2177	N	THR	1761	24.181	-21.031	17.004	1.00	49.32
ATOM	2178	CA	THR	1761	24.791	-20.166	17.987	1.00	50.15

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ATOM	2179	CB	THR	1761	24.309	-18.707	17.811	1.00	49.78
ATOM	2180	OG1	THR	1761	24.650	-18.262	16.489	1.00	49.83
ATOM	2181	CG2	THR	1761	24.997	-17.793	18.809	1.00	49.37
ATOM	2182	C	THR	1761	24.643	-20.655	19.426	1.00	51.84
ATOM	2183	O	THR	1761	23.565	-21.064	19.866	1.00	51.38
ATOM	2184	N	SER	1762	25.761	-20.622	20.143	1.00	53.45
ATOM	2185	CA	SER	1762	25.835	-21.042	21.533	1.00	53.79
ATOM	2186	CB	SER	1762	27.301	-21.039	21.969	1.00	58.33
ATOM	2187	OG	SER	1762	27.502	-21.759	23.173	1.00	63.27
ATOM	2188	C	SER	1762	25.033	-20.081	22.403	1.00	50.43
ATOM	2189	O	SER	1762	25.193	-18.856	22.301	1.00	48.42
ATOM	2190	N	ALA	461	79.680	25.808	14.502	1.00	57.40
ATOM	2191	CA	ALA	461	79.609	24.651	13.610	1.00	53.47
ATOM	2192	CB	ALA	461	78.307	23.875	13.860	1.00	54.34
ATOM	2193	C	ALA	461	79.707	25.105	12.151	1.00	49.53
ATOM	2194	O	ALA	461	79.739	24.289	11.243	1.00	48.04
ATOM	2195	N	ALA	462	79.814	26.417	11.957	1.00	46.57
ATOM	2196	CA	ALA	462	79.919	27.014	10.634	1.00	43.66
ATOM	2197	CB	ALA	462	80.034	28.532	10.750	1.00	43.87
ATOM	2198	C	ALA	462	81.074	26.461	9.806	1.00	39.75
ATOM	2199	O	ALA	462	80.869	26.036	8.673	1.00	36.18
ATOM	2200	N	TYR	463	82.279	26.449	10.383	1.00	37.82
ATOM	2201	CA	TYR	463	83.477	25.959	9.686	1.00	36.88
ATOM	2202	CB	TYR	463	84.615	26.968	9.765	1.00	39.12
ATOM	2203	CG	TYR	463	84.372	28.176	8.894	1.00	45.68
ATOM	2204	CD1	TYR	463	84.071	29.422	9.456	1.00	46.07
ATOM	2205	CE1	TYR	463	83.783	30.518	8.652	1.00	48.07
ATOM	2206	CD2	TYR	463	84.384	28.064	7.501	1.00	47.80
ATOM	2207	CE2	TYR	463	84.096	29.154	6.690	1.00	45.55
ATOM	2208	CZ	TYR	463	83.796	30.372	7.271	1.00	47.44
ATOM	2209	OH	TYR	463	83.491	31.442	6.476	1.00	49.77
ATOM	2210	C	TYR	463	83.988	24.579	10.024	1.00	34.97
ATOM	2211	O	TYR	463	84.605	23.947	9.175	1.00	35.48
ATOM	2212	N	GLU	464	83.761	24.109	11.244	1.00	34.33
ATOM	2213	CA	GLU	464	84.224	22.769	11.630	1.00	36.96
ATOM	2214	CB	GLU	464	85.725	22.790	11.901	1.00	41.01
ATOM	2215	CG	GLU	464	86.123	23.764	12.991	1.00	45.91
ATOM	2216	CD	GLU	464	87.619	24.009	13.075	1.00	53.97
ATOM	2217	OE1	GLU	464	88.013	24.922	13.835	1.00	58.84
ATOM	2218	OE2	GLU	464	88.400	23.311	12.383	1.00	56.78
ATOM	2219	C	GLU	464	83.517	22.294	12.875	1.00	34.98
ATOM	2220	O	GLU	464	83.252	23.106	13.763	1.00	35.30
ATOM	2221	N	LEU	465	83.193	21.003	12.939	1.00	33.52
ATOM	2222	CA	LEU	465	82.527	20.449	14.121	1.00	35.65
ATOM	2223	CB	LEU	465	81.520	19.348	13.762	1.00	32.97
ATOM	2224	CG	LEU	465	80.488	19.538	12.651	1.00	33.16
ATOM	2225	CD1	LEU	465	79.356	18.544	12.911	1.00	27.30
ATOM	2226	CD2	LEU	465	79.983	20.981	12.596	1.00	29.96
ATOM	2227	C	LEU	465	83.572	19.862	15.058	1.00	38.14
ATOM	2228	O	LEU	465	84.707	19.573	14.642	1.00	35.58
ATOM	2229	N	PRO	466	83.215	19.684	16.338	1.00	39.91
ATOM	2230	CD	PRO	466	81.929	20.073	16.942	1.00	42.38

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ATOM	2231	CA	PRO	466	84.118	19.126	17.348	1.00	40.82
ATOM	2232	CB	PRO	466	83.264	19.131	18.611	1.00	41.62
ATOM	2233	CG	PRO	466	82.327	20.294	18.380	1.00	45.42
ATOM	2234	C	PRO	466	84.475	17.707	16.976	1.00	41.29
ATOM	2235	O	PRO	466	83.681	16.996	16.361	1.00	40.64
ATOM	2236	N	GLU	467	85.664	17.292	17.370	1.00	43.54
ATOM	2237	CA	GLU	467	86.106	15.950	17.065	1.00	47.01
ATOM	2238	CB	GLU	467	87.569	15.955	16.627	1.00	50.95
ATOM	2239	CG	GLU	467	88.000	14.641	15.990	1.00	59.47
ATOM	2240	CD	GLU	467	89.372	14.700	15.334	1.00	63.95
ATOM	2241	OE1	GLU	467	90.123	15.688	15.538	1.00	62.08
ATOM	2242	OE2	GLU	467	89.697	13.736	14.606	1.00	66.76
ATOM	2243	C	GLU	467	85.892	14.993	18.233	1.00	44.81
ATOM	2244	O	GLU	467	85.988	15.386	19.397	1.00	45.53
ATOM	2245	N	ASP	468	85.572	13.751	17.906	1.00	43.85
ATOM	2246	CA	ASP	468	85.357	12.708	18.903	1.00	43.44
ATOM	2247	CB	ASP	468	83.872	12.582	19.247	1.00	43.33
ATOM	2248	CG	ASP	468	83.611	11.659	20.420	1.00	44.52
ATOM	2249	OD1	ASP	468	82.452	11.613	20.888	1.00	48.19
ATOM	2250	OD2	ASP	468	84.557	10.985	20.877	1.00	42.43
ATOM	2251	C	ASP	468	85.887	11.411	18.299	1.00	42.37
ATOM	2252	O	ASP	468	85.158	10.644	17.669	1.00	43.22
ATOM	2253	N	PRO	469	87.194	11.182	18.433	1.00	40.72
ATOM	2254	CD	PRO	469	88.167	12.102	19.045	1.00	40.30
ATOM	2255	CA	PRO	469	87.861	9.992	17.909	1.00	39.00
ATOM	2256	CB	PRO	469	89.228	10.078	18.570	1.00	39.03
ATOM	2257	CG	PRO	469	89.484	11.564	18.551	1.00	38.11
ATOM	2258	C	PRO	469	87.173	8.663	18.229	1.00	39.37
ATOM	2259	O	PRO	469	87.235	7.718	17.442	1.00	39.27
ATOM	2260	N	ARG	470	86.497	8.596	19.371	1.00	39.93
ATOM	2261	CA	ARG	470	85.814	7.374	19.770	1.00	42.32
ATOM	2262	CB	ARG	470	85.030	7.614	21.062	1.00	46.12
ATOM	2263	CG	ARG	470	85.766	8.370	22.149	1.00	50.76
ATOM	2264	CD	ARG	470	84.839	8.592	23.344	1.00	52.76
ATOM	2265	NE	ARG	470	83.649	9.362	22.991	1.00	54.47
ATOM	2266	CZ	ARG	470	82.770	9.823	23.873	1.00	59.36
ATOM	2267	NH1	ARG	470	82.945	9.597	25.169	1.00	61.19
ATOM	2268	NH2	ARG	470	81.712	10.508	23.455	1.00	62.88
ATOM	2269	C	ARG	470	84.814	6.896	18.721	1.00	42.79
ATOM	2270	O	ARG	470	84.670	5.700	18.504	1.00	45.63
ATOM	2271	N	TRP	471	84.139	7.844	18.078	1.00	41.98
ATOM	2272	CA	TRP	471	83.100	7.542	17.093	1.00	38.34
ATOM	2273	CB	TRP	471	81.844	8.307	17.451	1.00	35.68
ATOM	2274	CG	TRP	471	81.195	7.794	18.670	1.00	37.42
ATOM	2275	CD2	TRP	471	80.388	6.614	18.772	1.00	37.19
ATOM	2276	CE2	TRP	471	79.961	6.513	20.112	1.00	36.99
ATOM	2277	CE3	TRP	471	79.987	5.626	17.855	1.00	37.80
ATOM	2278	CD1	TRP	471	81.223	8.350	19.923	1.00	33.34
ATOM	2279	NE1	TRP	471	80.486	7.583	20.794	1.00	34.46
ATOM	2280	CZ2	TRP	471	79.150	5.464	20.559	1.00	38.31
ATOM	2281	CZ3	TRP	471	79.180	4.578	18.303	1.00	36.97
ATOM	2282	CH2	TRP	471	78.772	4.506	19.638	1.00	36.14

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ATOM	2283	C	TRP	471	83.409	7.830	15.641	1.00	38.26
ATOM	2284	O	TRP	471	82.655	7.430	14.749	1.00	38.72
ATOM	2285	N	GLU	472	84.478	8.569	15.397	1.00	37.71
ATOM	2286	CA	GLU	472	84.839	8.951	14.041	1.00	38.43
ATOM	2287	CB	GLU	472	86.014	9.924	14.087	1.00	37.56
ATOM	2288	CG	GLU	472	86.146	10.835	12.871	1.00	37.26
ATOM	2289	CD	GLU	472	84.930	11.728	12.625	1.00	39.02
ATOM	2290	OE1	GLU	472	84.361	12.301	13.571	1.00	40.26
ATOM	2291	OE2	GLU	472	84.568	11.879	11.445	1.00	39.35
ATOM	2292	C	GLU	472	85.135	7.806	13.069	1.00	38.32
ATOM	2293	O	GLU	472	85.872	6.875	13.386	1.00	38.11
ATOM	2294	N	LEU	473	84.535	7.884	11.883	1.00	38.44
ATOM	2295	CA	LEU	473	84.775	6.893	10.848	1.00	37.19
ATOM	2296	CB	LEU	473	83.505	6.112	10.511	1.00	35.38
ATOM	2297	CG	LEU	473	83.805	4.910	9.599	1.00	36.49
ATOM	2298	CD1	LEU	473	84.365	3.748	10.406	1.00	34.47
ATOM	2299	CD2	LEU	473	82.556	4.452	8.859	1.00	37.55
ATOM	2300	C	LEU	473	85.283	7.623	9.601	1.00	38.21
ATOM	2301	O	LEU	473	84.696	8.631	9.187	1.00	38.52
ATOM	2302	N	PRO	474	86.412	7.156	9.025	1.00	37.74
ATOM	2303	CD	PRO	474	87.292	6.107	9.568	1.00	36.38
ATOM	2304	CA	PRO	474	87.010	7.753	7.824	1.00	36.91
ATOM	2305	CB	PRO	474	88.233	6.865	7.587	1.00	34.65
ATOM	2306	CG	PRO	474	88.620	6.477	8.967	1.00	32.99
ATOM	2307	C	PRO	474	86.036	7.663	6.660	1.00	38.15
ATOM	2308	O	PRO	474	85.536	6.578	6.362	1.00	38.24
ATOM	2309	N	ARG	475	85.793	8.784	5.981	1.00	38.90
ATOM	2310	CA	ARG	475	84.846	8.802	4.863	1.00	41.23
ATOM	2311	CB	ARG	475	84.743	10.206	4.258	1.00	38.36
ATOM	2312	CG	ARG	475	84.311	11.271	5.267	1.00	35.30
ATOM	2313	CD	ARG	475	84.282	12.691	4.679	1.00	35.23
ATOM	2314	NE	ARG	475	83.850	13.658	5.679	1.00	27.27
ATOM	2315	CZ	ARG	475	82.585	13.859	6.011	1.00	25.77
ATOM	2316	NH1	ARG	475	81.630	13.181	5.402	1.00	25.09
ATOM	2317	NH2	ARG	475	82.286	14.639	7.047	1.00	25.24
ATOM	2318	C	ARG	475	85.101	7.745	3.791	1.00	42.43
ATOM	2319	O	ARG	475	84.160	7.212	3.204	1.00	44.06
ATOM	2320	N	ASP	476	86.359	7.381	3.594	1.00	44.69
ATOM	2321	CA	ASP	476	86.690	6.384	2.583	1.00	48.37
ATOM	2322	CB	ASP	476	88.197	6.371	2.319	1.00	52.12
ATOM	2323	CG	ASP	476	88.988	5.925	3.521	1.00	56.56
ATOM	2324	OD1	ASP	476	89.299	4.718	3.613	1.00	59.72
ATOM	2325	OD2	ASP	476	89.294	6.779	4.376	1.00	61.19
ATOM	2326	C	ASP	476	86.210	4.988	2.973	1.00	49.50
ATOM	2327	O	ASP	476	86.204	4.074	2.145	1.00	51.61
ATOM	2328	N	ARG	477	85.852	4.814	4.241	1.00	48.26
ATOM	2329	CA	ARG	477	85.357	3.525	4.732	1.00	47.16
ATOM	2330	CB	ARG	477	85.909	3.252	6.126	1.00	49.76
ATOM	2331	CG	ARG	477	87.325	2.723	6.088	1.00	53.26
ATOM	2332	CD	ARG	477	88.043	2.898	7.406	1.00	58.02
ATOM	2333	NE	ARG	477	87.394	2.213	8.517	1.00	61.16
ATOM	2334	CZ	ARG	477	87.810	2.297	9.776	1.00	63.35

ATOM	2335	NH1	ARG	477	88.875	3.032	10.081	1.00	64.92
ATOM	2336	NH2	ARG	477	87.139	1.675	10.738	1.00	66.00
ATOM	2337	C	ARG	477	83.822	3.445	4.740	1.00	45.38
ATOM	2338	O	ARG	477	83.239	2.540	5.336	1.00	43.67
ATOM	2339	N	LEU	478	83.175	4.364	4.026	1.00	42.09
ATOM	2340	CA	LEU	478	81.721	4.410	3.951	1.00	37.74
ATOM	2341	CB	LEU	478	81.198	5.539	4.849	1.00	32.19
ATOM	2342	CG	LEU	478	79.673	5.638	4.973	1.00	30.21
ATOM	2343	CD1	LEU	478	79.146	4.635	5.983	1.00	22.82
ATOM	2344	CD2	LEU	478	79.313	7.035	5.422	1.00	34.82
ATOM	2345	C	LEU	478	81.329	4.702	2.514	1.00	38.75
ATOM	2346	O	LEU	478	81.818	5.669	1.935	1.00	40.60
ATOM	2347	N	VAL	479	80.477	3.863	1.925	1.00	38.78
ATOM	2348	CA	VAL	479	80.020	4.058	0.544	1.00	37.97
ATOM	2349	CB	VAL	479	80.353	2.845	-0.360	1.00	36.36
ATOM	2350	CG1	VAL	479	79.837	3.090	-1.759	1.00	33.55
ATOM	2351	CG2	VAL	479	81.868	2.626	-0.405	1.00	33.76
ATOM	2352	C	VAL	479	78.523	4.298	0.562	1.00	37.83
ATOM	2353	O	VAL	479	77.750	3.383	0.820	1.00	37.70
ATOM	2354	N	LEU	480	78.127	5.542	0.305	1.00	39.32
ATOM	2355	CA	LEU	480	76.723	5.942	0.333	1.00	38.41
ATOM	2356	CB	LEU	480	76.630	7.458	0.224	1.00	38.29
ATOM	2357	CG	LEU	480	77.287	8.226	1.377	1.00	37.99
ATOM	2358	CD1	LEU	480	77.098	9.730	1.159	1.00	34.00
ATOM	2359	CD2	LEU	480	76.666	7.785	2.703	1.00	32.79
ATOM	2360	C	LEU	480	75.893	5.287	-0.753	1.00	38.24
ATOM	2361	O	LEU	480	76.315	5.205	-1.903	1.00	39.11
ATOM	2362	N	GLY	481	74.672	4.896	-0.394	1.00	36.70
ATOM	2363	CA	GLY	481	73.811	4.223	-1.357	1.00	36.53
ATOM	2364	C	GLY	481	72.417	4.782	-1.524	1.00	37.61
ATOM	2365	O	GLY	481	72.159	5.961	-1.277	1.00	40.02
ATOM	2366	N	LYS	482	71.484	3.913	-1.911	1.00	37.52
ATOM	2367	CA	LYS	482	70.099	4.313	-2.153	1.00	39.89
ATOM	2368	CB	LYS	482	69.243	3.104	-2.551	1.00	42.44
ATOM	2369	C	LYS	482	69.447	5.028	-0.984	1.00	41.25
ATOM	2370	O	LYS	482	69.538	4.589	0.163	1.00	42.22
ATOM	2371	N	PRO	483	68.779	6.156	-1.263	1.00	41.71
ATOM	2372	CD	PRO	483	68.643	6.876	-2.537	1.00	41.01
ATOM	2373	CA	PRO	483	68.118	6.889	-0.193	1.00	42.72
ATOM	2374	CB	PRO	483	67.606	8.146	-0.906	1.00	41.26
ATOM	2375	CG	PRO	483	67.425	7.713	-2.290	1.00	40.16
ATOM	2376	C	PRO	483	66.999	6.061	0.429	1.00	44.69
ATOM	2377	O	PRO	483	66.306	5.314	-0.262	1.00	45.26
ATOM	2378	N	LEU	484	66.883	6.163	1.751	1.00	45.34
ATOM	2379	CA	LEU	484	65.872	5.450	2.512	1.00	47.34
ATOM	2380	CB	LEU	484	66.494	4.793	3.746	1.00	42.40
ATOM	2381	CG	LEU	484	67.517	3.668	3.535	1.00	39.50
ATOM	2382	CD1	LEU	484	68.208	3.337	4.828	1.00	33.64
ATOM	2383	CD2	LEU	484	66.861	2.419	3.003	1.00	33.44
ATOM	2384	C	LEU	484	64.733	6.391	2.927	1.00	52.14
ATOM	2385	O	LEU	484	63.611	5.941	3.142	1.00	53.64
ATOM	2386	N	GLY	485	65.013	7.697	3.025	1.00	55.25

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ATOM	2387	CA	GLY	485	63.982	8.653	3.427	1.00	58.76
ATOM	2388	C	GLY	485	64.441	10.104	3.503	1.00	60.58
ATOM	2389	O	GLY	485	65.640	10.376	3.600	1.00	61.49
ATOM	2390	N	ALA	486	63.490	11.032	3.489	1.00	61.46
ATOM	2391	CA	ALA	486	63.791	12.458	3.545	1.00	63.24
ATOM	2392	CB	ALA	486	63.847	13.035	2.126	1.00	64.42
ATOM	2393	C	ALA	486	62.730	13.179	4.355	1.00	63.86
ATOM	2394	O	ALA	486	61.655	12.633	4.599	1.00	65.24
ATOM	2395	N	GLY	487	63.022	14.404	4.768	1.00	63.89
ATOM	2396	CA	GLY	487	62.054	15.158	5.538	1.00	64.30
ATOM	2397	C	GLY	487	62.431	16.617	5.623	1.00	65.34
ATOM	2398	O	GLY	487	63.071	17.154	4.718	1.00	65.98
ATOM	2399	N	ALA	488	62.023	17.259	6.711	1.00	66.16
ATOM	2400	CA	ALA	488	62.317	18.666	6.934	1.00	66.71
ATOM	2401	CB	ALA	488	61.647	19.132	8.219	1.00	70.05
ATOM	2402	C	ALA	488	63.828	18.844	7.027	1.00	66.55
ATOM	2403	O	ALA	488	64.432	18.547	8.063	1.00	65.59
ATOM	2404	N	PHE	489	64.430	19.228	5.904	1.00	65.54
ATOM	2405	CA	PHE	489	65.875	19.457	5.807	1.00	65.40
ATOM	2406	CB	PHE	489	66.244	20.775	6.498	1.00	67.06
ATOM	2407	C	PHE	489	66.773	18.296	6.311	1.00	64.01
ATOM	2408	O	PHE	489	67.942	18.502	6.651	1.00	62.51
ATOM	2409	N	GLY	490	66.234	17.075	6.288	1.00	61.41
ATOM	2410	CA	GLY	490	66.974	15.901	6.724	1.00	55.89
ATOM	2411	C	GLY	490	66.858	14.821	5.667	1.00	53.58
ATOM	2412	O	GLY	490	65.825	14.703	5.000	1.00	54.22
ATOM	2413	N	GLN	491	67.899	14.006	5.543	1.00	51.23
ATOM	2414	CA	GLN	491	67.966	12.934	4.556	1.00	47.90
ATOM	2415	CB	GLN	491	68.823	13.445	3.387	1.00	50.09
ATOM	2416	CG	GLN	491	68.979	12.529	2.183	1.00	56.77
ATOM	2417	CD	GLN	491	69.945	13.115	1.161	1.00	60.83
ATOM	2418	OE1	GLN	491	70.283	14.292	1.218	1.00	65.11
ATOM	2419	NE2	GLN	491	70.411	12.284	0.232	1.00	63.81
ATOM	2420	C	GLN	491	68.597	11.673	5.190	1.00	45.27
ATOM	2421	O	GLN	491	69.507	11.758	6.014	1.00	45.41
ATOM	2422	N	VAL	492	68.112	10.503	4.805	1.00	41.69
ATOM	2423	CA	VAL	492	68.624	9.245	5.325	1.00	39.95
ATOM	2424	CB	VAL	492	67.583	8.528	6.230	1.00	41.77
ATOM	2425	CG1	VAL	492	68.117	7.168	6.701	1.00	39.86
ATOM	2426	CG2	VAL	492	67.226	9.399	7.421	1.00	42.87
ATOM	2427	C	VAL	492	68.911	8.348	4.126	1.00	38.86
ATOM	2428	O	VAL	492	68.025	8.114	3.301	1.00	37.55
ATOM	2429	N	VAL	493	70.141	7.862	4.010	1.00	36.01
ATOM	2430	CA	VAL	493	70.481	6.994	2.895	1.00	37.55
ATOM	2431	CB	VAL	493	71.471	7.674	1.889	1.00	38.65
ATOM	2432	CG1	VAL	493	71.128	9.137	1.709	1.00	37.08
ATOM	2433	CG2	VAL	493	72.929	7.498	2.318	1.00	39.03
ATOM	2434	C	VAL	493	71.071	5.678	3.371	1.00	38.61
ATOM	2435	O	VAL	493	71.645	5.599	4.456	1.00	39.75
ATOM	2436	N	LEU	494	70.899	4.637	2.572	1.00	39.68
ATOM	2437	CA	LEU	494	71.460	3.345	2.910	1.00	40.98
ATOM	2438	CB	LEU	494	70.748	2.241	2.123	1.00	42.14

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ATOM	2439	CG	LEU	494	71.250	0.808	2.305	1.00	40.33
ATOM	2440	CD1	LEU	494	71.186	0.425	3.765	1.00	39.62
ATOM	2441	CD2	LEU	494	70.411	-0.117	1.459	1.00	40.75
ATOM	2442	C	LEU	494	72.918	3.432	2.483	1.00	40.66
ATOM	2443	O	LEU	494	73.249	4.163	1.552	1.00	40.05
ATOM	2444	N	ALA	495	73.798	2.725	3.169	1.00	39.74
ATOM	2445	CA	ALA	495	75.202	2.768	2.820	1.00	42.06
ATOM	2446	CB	ALA	495	75.858	3.999	3.468	1.00	42.91
ATOM	2447	C	ALA	495	75.887	1.497	3.289	1.00	43.34
ATOM	2448	O	ALA	495	75.271	0.668	3.946	1.00	43.81
ATOM	2449	N	GLU	496	77.140	1.314	2.880	1.00	44.40
ATOM	2450	CA	GLU	496	77.910	0.154	3.297	1.00	45.12
ATOM	2451	CB	GLU	496	78.282	-0.722	2.106	1.00	48.62
ATOM	2452	CG	GLU	496	77.062	-1.206	1.346	1.00	56.98
ATOM	2453	CD	GLU	496	77.316	-2.476	0.567	1.00	60.32
ATOM	2454	OE1	GLU	496	76.448	-3.378	0.634	1.00	62.17
ATOM	2455	OE2	GLU	496	78.371	-2.575	-0.103	1.00	60.48
ATOM	2456	C	GLU	496	79.151	0.658	3.987	1.00	43.27
ATOM	2457	O	GLU	496	79.957	1.366	3.387	1.00	44.49
ATOM	2458	N	ALA	497	79.232	0.385	5.282	1.00	43.29
ATOM	2459	CA	ALA	497	80.374	0.799	6.086	1.00	44.01
ATOM	2460	CB	ALA	497	79.910	1.182	7.471	1.00	42.35
ATOM	2461	C	ALA	497	81.381	-0.351	6.150	1.00	45.60
ATOM	2462	O	ALA	497	80.997	-1.512	6.107	1.00	43.35
ATOM	2463	N	ILE	498	82.666	-0.025	6.206	1.00	48.78
ATOM	2464	CA	ILE	498	83.709	-1.042	6.262	1.00	49.43
ATOM	2465	CB	ILE	498	84.611	-0.977	5.014	1.00	50.66
ATOM	2466	CG2	ILE	498	85.681	-2.054	5.082	1.00	51.85
ATOM	2467	CG1	ILE	498	83.780	-1.150	3.741	1.00	50.27
ATOM	2468	CD1	ILE	498	83.073	0.112	3.255	1.00	54.24
ATOM	2469	C	ILE	498	84.572	-0.878	7.510	1.00	50.32
ATOM	2470	O	ILE	498	85.055	0.219	7.801	1.00	49.08
ATOM	2471	N	GLY	499	84.713	-1.964	8.270	1.00	51.88
ATOM	2472	CA	GLY	499	85.526	-1.958	9.480	1.00	55.86
ATOM	2473	C	GLY	499	85.061	-1.111	10.661	1.00	59.72
ATOM	2474	O	GLY	499	85.885	-0.545	11.393	1.00	61.66
ATOM	2475	N	LEU	500	83.747	-1.058	10.878	1.00	59.88
ATOM	2476	CA	LEU	500	83.167	-0.275	11.974	1.00	58.62
ATOM	2477	CB	LEU	500	81.663	-0.556	12.086	1.00	57.41
ATOM	2478	CG	LEU	500	80.764	-0.090	10.937	1.00	55.24
ATOM	2479	CD1	LEU	500	79.331	-0.536	11.168	1.00	51.91
ATOM	2480	CD2	LEU	500	80.845	1.426	10.799	1.00	54.93
ATOM	2481	C	LEU	500	83.849	-0.565	13.306	1.00	58.51
ATOM	2482	O	LEU	500	84.226	-1.710	13.576	1.00	60.71
ATOM	2483	N	PRO	505	87.501	-6.102	10.460	1.00	82.25
ATOM	2484	CD	PRO	505	88.578	-6.722	11.248	1.00	82.69
ATOM	2485	CA	PRO	505	87.860	-4.730	10.077	1.00	80.47
ATOM	2486	CB	PRO	505	89.257	-4.557	10.686	1.00	80.88
ATOM	2487	CG	PRO	505	89.782	-5.960	10.770	1.00	81.84
ATOM	2488	C	PRO	505	87.850	-4.508	8.567	1.00	77.40
ATOM	2489	O	PRO	505	88.038	-3.391	8.087	1.00	76.83
ATOM	2490	N	ASN	506	87.632	-5.584	7.826	1.00	74.91

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ATOM	2491	CA	ASN	506	87.572	-5.502	6.375	1.00	73.04
ATOM	2492	CB	ASN	506	88.632	-6.406	5.749	1.00	73.39
ATOM	2493	C	ASN	506	86.180	-5.938	5.929	1.00	71.75
ATOM	2494	O	ASN	506	85.918	-6.094	4.739	1.00	71.33
ATOM	2495	N	ARG	507	85.294	-6.124	6.905	1.00	69.66
ATOM	2496	CA	ARG	507	83.924	-6.534	6.638	1.00	66.59
ATOM	2497	CB	ARG	507	83.369	-7.329	7.819	1.00	69.86
ATOM	2498	C	ARG	507	83.048	-5.321	6.409	1.00	63.59
ATOM	2499	O	ARG	507	83.225	-4.291	7.070	1.00	64.09
ATOM	2500	N	VAL	508	82.126	-5.429	5.462	1.00	59.52
ATOM	2501	CA	VAL	508	81.217	-4.334	5.187	1.00	57.28
ATOM	2502	CB	VAL	508	80.905	-4.178	3.686	1.00	55.73
ATOM	2503	CG1	VAL	508	82.163	-3.952	2.922	1.00	57.01
ATOM	2504	CG2	VAL	508	80.184	-5.390	3.149	1.00	58.06
ATOM	2505	C	VAL	508	79.928	-4.614	5.935	1.00	57.10
ATOM	2506	O	VAL	508	79.483	-5.759	6.018	1.00	57.35
ATOM	2507	N	THR	509	79.345	-3.555	6.482	1.00	55.31
ATOM	2508	CA	THR	509	78.107	-3.652	7.227	1.00	50.14
ATOM	2509	CB	THR	509	78.329	-3.192	8.686	1.00	50.91
ATOM	2510	OG1	THR	509	79.476	-3.851	9.227	1.00	49.20
ATOM	2511	CG2	THR	509	77.123	-3.524	9.559	1.00	51.96
ATOM	2512	C	THR	509	77.140	-2.705	6.528	1.00	47.53
ATOM	2513	O	THR	509	77.485	-1.558	6.242	1.00	47.22
ATOM	2514	N	LYS	510	75.958	-3.191	6.191	1.00	45.64
ATOM	2515	CA	LYS	510	74.975	-2.333	5.551	1.00	44.44
ATOM	2516	CB	LYS	510	73.861	-3.175	4.948	1.00	46.74
ATOM	2517	CG	LYS	510	73.008	-2.420	3.950	1.00	54.51
ATOM	2518	CD	LYS	510	73.463	-2.645	2.513	1.00	54.97
ATOM	2519	CE	LYS	510	72.846	-3.917	1.934	1.00	58.25
ATOM	2520	NZ	LYS	510	73.112	-5.150	2.740	1.00	58.33
ATOM	2521	C	LYS	510	74.430	-1.470	6.696	1.00	42.75
ATOM	2522	O	LYS	510	74.053	-2.006	7.742	1.00	43.14
ATOM	2523	N	VAL	511	74.443	-0.149	6.531	1.00	38.63
ATOM	2524	CA	VAL	511	73.975	0.757	7.576	1.00	34.16
ATOM	2525	CB	VAL	511	75.161	1.399	8.333	1.00	35.66
ATOM	2526	CG1	VAL	511	75.922	0.340	9.100	1.00	31.46
ATOM	2527	CG2	VAL	511	76.098	2.100	7.357	1.00	35.08
ATOM	2528	C	VAL	511	73.116	1.873	7.024	1.00	31.58
ATOM	2529	O	VAL	511	72.962	1.984	5.818	1.00	33.18
ATOM	2530	N	ALA	512	72.542	2.687	7.906	1.00	30.77
ATOM	2531	CA	ALA	512	71.724	3.818	7.484	1.00	28.58
ATOM	2532	CB	ALA	512	70.382	3.774	8.145	1.00	26.09
ATOM	2533	C	ALA	512	72.487	5.075	7.905	1.00	29.94
ATOM	2534	O	ALA	512	72.996	5.151	9.031	1.00	29.90
ATOM	2535	N	VAL	513	72.556	6.057	7.012	1.00	28.68
ATOM	2536	CA	VAL	513	73.286	7.290	7.280	1.00	28.26
ATOM	2537	CB	VAL	513	74.439	7.503	6.269	1.00	26.92
ATOM	2538	CG1	VAL	513	75.213	8.730	6.618	1.00	25.26
ATOM	2539	CG2	VAL	513	75.353	6.308	6.238	1.00	25.10
ATOM	2540	C	VAL	513	72.383	8.526	7.230	1.00	29.54
ATOM	2541	O	VAL	513	71.745	8.799	6.200	1.00	28.56
ATOM	2542	N	LYS	514	72.304	9.228	8.359	1.00	28.94

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ATOM	2543	CA	LYS	514	71.519	10.450	8.481	1.00	28.60
ATOM	2544	CB	LYS	514	70.942	10.611	9.893	1.00	31.19
ATOM	2545	CG	LYS	514	69.988	9.542	10.328	1.00	31.41
ATOM	2546	CD	LYS	514	69.454	9.922	11.690	1.00	40.14
ATOM	2547	CE	LYS	514	68.484	8.892	12.222	1.00	48.93
ATOM	2548	NZ	LYS	514	67.198	8.861	11.475	1.00	57.07
ATOM	2549	C	LYS	514	72.430	11.636	8.196	1.00	25.53
ATOM	2550	O	LYS	514	73.544	11.714	8.722	1.00	20.42
ATOM	2551	N	MET	515	71.928	12.576	7.407	1.00	26.63
ATOM	2552	CA	MET	515	72.676	13.762	7.008	1.00	27.59
ATOM	2553	CB	MET	515	73.425	13.487	5.693	1.00	28.22
ATOM	2554	CG	MET	515	72.502	13.026	4.556	1.00	28.70
ATOM	2555	SD	MET	515	73.377	12.418	3.113	1.00	32.30
ATOM	2556	CE	MET	515	73.949	10.803	3.715	1.00	24.88
ATOM	2557	C	MET	515	71.683	14.880	6.779	1.00	28.41
ATOM	2558	O	MET	515	70.472	14.685	6.889	1.00	32.15
ATOM	2559	N	LEU	516	72.202	16.056	6.466	1.00	29.12
ATOM	2560	CA	LEU	516	71.383	17.220	6.180	1.00	29.98
ATOM	2561	CB	LEU	516	72.110	18.512	6.593	1.00	25.32
ATOM	2562	CG	LEU	516	72.455	18.767	8.067	1.00	26.60
ATOM	2563	CD1	LEU	516	73.210	20.057	8.190	1.00	24.56
ATOM	2564	CD2	LEU	516	71.217	18.844	8.900	1.00	22.75
ATOM	2565	C	LEU	516	71.092	17.274	4.674	1.00	31.50
ATOM	2566	O	LEU	516	71.763	16.636	3.873	1.00	32.97
ATOM	2567	N	LYS	517	70.069	18.018	4.293	1.00	33.29
ATOM	2568	CA	LYS	517	69.755	18.187	2.890	1.00	32.20
ATOM	2569	CB	LYS	517	68.246	18.363	2.699	1.00	36.34
ATOM	2570	CG	LYS	517	67.432	17.182	3.192	1.00	43.49
ATOM	2571	CD	LYS	517	66.172	16.940	2.356	1.00	53.91
ATOM	2572	CE	LYS	517	65.088	17.984	2.581	1.00	58.71
ATOM	2573	NZ	LYS	517	63.902	17.740	1.704	1.00	59.37
ATOM	2574	C	LYS	517	70.520	19.455	2.507	1.00	31.31
ATOM	2575	O	LYS	517	70.917	20.217	3.383	1.00	28.74
ATOM	2576	N	SER	518	70.744	19.672	1.213	1.00	32.48
ATOM	2577	CA	SER	518	71.486	20.840	0.714	1.00	33.52
ATOM	2578	CB	SER	518	71.611	20.772	-0.809	1.00	32.98
ATOM	2579	OG	SER	518	70.375	20.407	-1.396	1.00	36.75
ATOM	2580	C	SER	518	70.896	22.189	1.110	1.00	34.62
ATOM	2581	O	SER	518	71.580	23.214	1.058	1.00	34.57
ATOM	2582	N	ASP	519	69.624	22.193	1.485	1.00	35.47
ATOM	2583	CA	ASP	519	68.943	23.422	1.885	1.00	36.10
ATOM	2584	CB	ASP	519	67.529	23.480	1.268	1.00	38.11
ATOM	2585	CG	ASP	519	66.668	22.258	1.608	1.00	41.64
ATOM	2586	OD1	ASP	519	67.150	21.309	2.253	1.00	41.70
ATOM	2587	OD2	ASP	519	65.478	22.250	1.220	1.00	49.25
ATOM	2588	C	ASP	519	68.881	23.645	3.395	1.00	34.66
ATOM	2589	O	ASP	519	68.266	24.602	3.860	1.00	33.39
ATOM	2590	N	ALA	520	69.551	22.784	4.150	1.00	33.52
ATOM	2591	CA	ALA	520	69.561	22.895	5.605	1.00	32.12
ATOM	2592	CB	ALA	520	70.253	21.687	6.207	1.00	32.08
ATOM	2593	C	ALA	520	70.242	24.163	6.076	1.00	30.91
ATOM	2594	O	ALA	520	71.014	24.778	5.331	1.00	30.57

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ATOM	2595	N	THR	521	69.943	24.555	7.311	1.00	30.80
ATOM	2596	CA	THR	521	70.546	25.738	7.921	1.00	32.33
ATOM	2597	CB	THR	521	69.493	26.763	8.440	1.00	34.30
ATOM	2598	OG1	THR	521	68.817	26.242	9.598	1.00	35.14
ATOM	2599	CG2	THR	521	68.484	27.109	7.366	1.00	37.70
ATOM	2600	C	THR	521	71.418	25.312	9.098	1.00	33.11
ATOM	2601	O	THR	521	71.518	24.125	9.426	1.00	31.39
ATOM	2602	N	GLU	522	72.022	26.293	9.753	1.00	34.91
ATOM	2603	CA	GLU	522	72.882	26.048	10.901	1.00	39.44
ATOM	2604	CB	GLU	522	73.516	27.357	11.360	1.00	46.96
ATOM	2605	CG	GLU	522	74.550	27.220	12.488	1.00	59.20
ATOM	2606	CD	GLU	522	75.919	26.740	12.011	1.00	64.70
ATOM	2607	OE1	GLU	522	76.910	27.478	12.219	1.00	63.87
ATOM	2608	OE2	GLU	522	76.006	25.627	11.445	1.00	71.55
ATOM	2609	C	GLU	522	72.083	25.428	12.044	1.00	39.61
ATOM	2610	O	GLU	522	72.587	24.554	12.757	1.00	36.74
ATOM	2611	N	LYS	523	70.827	25.849	12.193	1.00	38.60
ATOM	2612	CA	LYS	523	69.970	25.327	13.252	1.00	37.77
ATOM	2613	CB	LYS	523	68.628	26.053	13.273	1.00	44.52
ATOM	2614	CG	LYS	523	67.665	25.562	14.355	1.00	51.14
ATOM	2615	CD	LYS	523	66.380	24.983	13.756	1.00	57.39
ATOM	2616	CE	LYS	523	65.499	24.376	14.852	1.00	59.17
ATOM	2617	NZ	LYS	523	64.365	23.553	14.327	1.00	62.68
ATOM	2618	C	LYS	523	69.751	23.849	13.002	1.00	34.63
ATOM	2619	O	LYS	523	69.817	23.041	13.931	1.00	35.00
ATOM	2620	N	ASP	524	69.496	23.495	11.746	1.00	31.60
ATOM	2621	CA	ASP	524	69.293	22.100	11.367	1.00	29.05
ATOM	2622	CB	ASP	524	69.002	21.975	9.871	1.00	29.60
ATOM	2623	CG	ASP	524	67.695	22.626	9.472	1.00	31.90
ATOM	2624	OD1	ASP	524	66.666	22.368	10.130	1.00	38.83
ATOM	2625	OD2	ASP	524	67.687	23.383	8.485	1.00	29.79
ATOM	2626	C	ASP	524	70.558	21.317	11.696	1.00	28.02
ATOM	2627	O	ASP	524	70.494	20.201	12.212	1.00	28.12
ATOM	2628	N	LEU	525	71.709	21.899	11.378	1.00	28.32
ATOM	2629	CA	LEU	525	72.971	21.231	11.677	1.00	27.71
ATOM	2630	CB	LEU	525	74.173	22.085	11.257	1.00	22.53
ATOM	2631	CG	LEU	525	75.548	21.490	11.602	1.00	22.13
ATOM	2632	CD1	LEU	525	75.677	20.082	11.019	1.00	19.92
ATOM	2633	CD2	LEU	525	76.673	22.401	11.147	1.00	18.60
ATOM	2634	C	LEU	525	73.007	20.952	13.162	1.00	27.44
ATOM	2635	O	LEU	525	73.227	19.817	13.577	1.00	29.73
ATOM	2636	N	SER	526	72.689	21.976	13.947	1.00	29.09
ATOM	2637	CA	SER	526	72.672	21.891	15.412	1.00	30.83
ATOM	2638	CB	SER	526	72.222	23.230	16.006	1.00	34.25
ATOM	2639	OG	SER	526	71.966	23.147	17.397	1.00	40.67
ATOM	2640	C	SER	526	71.765	20.777	15.931	1.00	29.32
ATOM	2641	O	SER	526	72.055	20.133	16.954	1.00	28.94
ATOM	2642	N	ASP	527	70.644	20.587	15.242	1.00	26.54
ATOM	2643	CA	ASP	527	69.681	19.558	15.601	1.00	27.00
ATOM	2644	CB	ASP	527	68.392	19.798	14.829	1.00	25.91
ATOM	2645	CG	ASP	527	67.640	21.052	15.290	1.00	29.22
ATOM	2646	OD1	ASP	527	68.016	21.662	16.320	1.00	26.80

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ATOM	2647	OD2	ASP	527	66.660	21.425	14.605	1.00	33.85
ATOM	2648	C	ASP	527	70.231	18.155	15.325	1.00	28.34
ATOM	2649	O	ASP	527	70.058	17.240	16.130	1.00	28.36
ATOM	2650	N	LEU	528	70.884	17.982	14.177	1.00	29.50
ATOM	2651	CA	LEU	528	71.448	16.680	13.830	1.00	30.48
ATOM	2652	CB	LEU	528	71.915	16.651	12.366	1.00	27.89
ATOM	2653	CG	LEU	528	72.443	15.305	11.832	1.00	26.48
ATOM	2654	CD1	LEU	528	71.468	14.154	12.148	1.00	21.52
ATOM	2655	CD2	LEU	528	72.722	15.383	10.333	1.00	20.23
ATOM	2656	C	LEU	528	72.583	16.308	14.804	1.00	31.69
ATOM	2657	O	LEU	528	72.688	15.145	15.222	1.00	30.09
ATOM	2658	N	ILE	529	73.397	17.298	15.195	1.00	30.79
ATOM	2659	CA	ILE	529	74.503	17.082	16.140	1.00	28.88
ATOM	2660	CB	ILE	529	75.398	18.310	16.278	1.00	25.69
ATOM	2661	CG2	ILE	529	76.541	18.007	17.217	1.00	20.54
ATOM	2662	CG1	ILE	529	75.960	18.727	14.941	1.00	23.71
ATOM	2663	CD1	ILE	529	76.981	19.831	15.035	1.00	24.21
ATOM	2664	C	ILE	529	73.951	16.767	17.533	1.00	31.52
ATOM	2665	O	ILE	529	74.439	15.850	18.213	1.00	30.66
ATOM	2666	N	SER	530	72.917	17.500	17.947	1.00	29.79
ATOM	2667	CA	SER	530	72.315	17.257	19.244	1.00	32.03
ATOM	2668	CB	SER	530	71.176	18.239	19.492	1.00	38.91
ATOM	2669	OG	SER	530	70.266	18.231	18.412	1.00	49.86
ATOM	2670	C	SER	530	71.795	15.819	19.316	1.00	30.10
ATOM	2671	O	SER	530	71.921	15.154	20.353	1.00	31.31
ATOM	2672	N	GLU	531	71.185	15.350	18.231	1.00	27.18
ATOM	2673	CA	GLU	531	70.671	13.989	18.180	1.00	27.89
ATOM	2674	CB	GLU	531	69.923	13.744	16.881	1.00	31.29
ATOM	2675	CG	GLU	531	69.434	12.324	16.769	1.00	30.43
ATOM	2676	CD	GLU	531	68.717	12.040	15.486	1.00	30.67
ATOM	2677	OE1	GLU	531	68.293	10.892	15.317	1.00	37.79
ATOM	2678	OE2	GLU	531	68.571	12.941	14.643	1.00	34.20
ATOM	2679	C	GLU	531	71.765	12.929	18.348	1.00	26.67
ATOM	2680	O	GLU	531	71.604	11.986	19.119	1.00	24.33
ATOM	2681	N	MET	532	72.851	13.074	17.595	1.00	28.93
ATOM	2682	CA	MET	532	74.000	12.156	17.644	1.00	28.35
ATOM	2683	CB	MET	532	75.073	12.637	16.659	1.00	29.48
ATOM	2684	CG	MET	532	76.458	12.034	16.827	1.00	25.84
ATOM	2685	SD	MET	532	77.650	12.692	15.582	1.00	30.60
ATOM	2686	CE	MET	532	77.831	14.373	16.151	1.00	20.10
ATOM	2687	C	MET	532	74.571	12.120	19.057	1.00	29.06
ATOM	2688	O	MET	532	74.876	11.053	19.589	1.00	28.22
ATOM	2689	N	GLU	533	74.640	13.289	19.688	1.00	28.61
ATOM	2690	CA	GLU	533	75.150	13.388	21.041	1.00	28.40
ATOM	2691	CB	GLU	533	75.340	14.846	21.429	1.00	29.34
ATOM	2692	CG	GLU	533	76.449	15.534	20.640	1.00	31.87
ATOM	2693	CD	GLU	533	77.822	14.923	20.892	1.00	35.10
ATOM	2694	OE1	GLU	533	78.242	14.831	22.067	1.00	37.36
ATOM	2695	OE2	GLU	533	78.490	14.543	19.913	1.00	37.71
ATOM	2696	C	GLU	533	74.211	12.684	22.023	1.00	31.03
ATOM	2697	O	GLU	533	74.651	11.936	22.906	1.00	30.76
ATOM	2698	N	MET	534	72.909	12.902	21.860	1.00	31.71

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ATOM	2699	CA	MET	534	71.940	12.256	22.727	1.00	30.58
ATOM	2700	CB	MET	534	70.510	12.620	22.315	1.00	33.53
ATOM	2701	CG	MET	534	69.538	12.624	23.509	0.50	32.45
ATOM	2702	SD	MET	534	67.778	12.682	23.150	0.50	30.95
ATOM	2703	CE	MET	534	67.523	14.422	22.895	0.50	30.50
ATOM	2704	C	MET	534	72.158	10.752	22.616	1.00	28.44
ATOM	2705	O	MET	534	72.304	10.077	23.614	1.00	27.63
ATOM	2706	N	MET	535	72.216	10.232	21.395	1.00	30.00
ATOM	2707	CA	MET	535	72.448	8.800	21.176	1.00	29.38
ATOM	2708	CB	MET	535	72.626	8.483	19.690	1.00	25.41
ATOM	2709	CG	MET	535	71.395	8.753	18.893	1.00	25.06
ATOM	2710	SD	MET	535	71.468	7.917	17.344	1.00	27.17
ATOM	2711	CE	MET	535	71.439	9.227	16.247	1.00	33.70
ATOM	2712	C	MET	535	73.675	8.345	21.938	1.00	30.77
ATOM	2713	O	MET	535	73.681	7.254	22.534	1.00	27.49
ATOM	2714	N	LYS	536	74.710	9.183	21.916	1.00	32.72
ATOM	2715	CA	LYS	536	75.937	8.889	22.649	1.00	34.05
ATOM	2716	CB	LYS	536	76.995	9.964	22.401	1.00	32.69
ATOM	2717	CG	LYS	536	77.719	9.838	21.073	1.00	28.00
ATOM	2718	CD	LYS	536	78.732	10.956	20.941	1.00	29.61
ATOM	2719	CE	LYS	536	79.242	11.124	19.514	1.00	26.58
ATOM	2720	NZ	LYS	536	80.020	12.389	19.460	1.00	22.22
ATOM	2721	C	LYS	536	75.652	8.769	24.145	1.00	34.80
ATOM	2722	O	LYS	536	76.004	7.763	24.750	1.00	34.44
ATOM	2723	N	MET	537	74.958	9.749	24.716	1.00	34.66
ATOM	2724	CA	MET	537	74.634	9.724	26.131	1.00	37.25
ATOM	2725	CB	MET	537	73.951	11.034	26.549	1.00	46.08
ATOM	2726	CG	MET	537	74.862	12.272	26.619	1.00	57.95
ATOM	2727	SD	MET	537	76.159	12.203	27.919	1.00	66.50
ATOM	2728	CE	MET	537	75.287	12.873	29.377	1.00	64.52
ATOM	2729	C	MET	537	73.749	8.537	26.523	1.00	36.05
ATOM	2730	O	MET	537	74.021	7.865	27.514	1.00	36.71
ATOM	2731	N	ILE	538	72.730	8.255	25.719	1.00	33.77
ATOM	2732	CA	ILE	538	71.804	7.160	26.007	1.00	30.52
ATOM	2733	CB	ILE	538	70.616	7.172	25.012	1.00	28.15
ATOM	2734	CG2	ILE	538	69.780	5.899	25.122	1.00	26.08
ATOM	2735	CG1	ILE	538	69.729	8.377	25.289	1.00	26.24
ATOM	2736	CD1	ILE	538	68.644	8.558	24.256	1.00	26.87
ATOM	2737	C	ILE	538	72.399	5.750	26.100	1.00	30.05
ATOM	2738	O	ILE	538	71.984	4.950	26.941	1.00	31.57
ATOM	2739	N	GLY	539	73.320	5.424	25.211	1.00	30.34
ATOM	2740	CA	GLY	539	73.910	4.103	25.249	1.00	28.22
ATOM	2741	C	GLY	539	73.158	3.094	24.408	1.00	31.25
ATOM	2742	O	GLY	539	72.050	3.359	23.935	1.00	32.88
ATOM	2743	N	LYS	540	73.781	1.933	24.221	1.00	31.96
ATOM	2744	CA	LYS	540	73.222	0.845	23.416	1.00	33.40
ATOM	2745	CB	LYS	540	74.342	-0.023	22.878	1.00	31.53
ATOM	2746	CG	LYS	540	75.177	0.645	21.846	1.00	37.05
ATOM	2747	CD	LYS	540	76.273	-0.266	21.361	1.00	40.15
ATOM	2748	CE	LYS	540	77.143	0.480	20.363	1.00	46.84
ATOM	2749	NZ	LYS	540	76.374	0.920	19.152	1.00	48.60
ATOM	2750	C	LYS	540	72.183	-0.090	24.023	1.00	36.22

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ATOM	2751	O	LYS	540	72.237	-0.430	25.215	1.00	40.10
ATOM	2752	N	HIS	541	71.254	-0.521	23.175	1.00	34.86
ATOM	2753	CA	HIS	541	70.223	-1.486	23.535	1.00	33.96
ATOM	2754	CB	HIS	541	69.064	-0.860	24.293	1.00	31.57
ATOM	2755	CG	HIS	541	68.127	-1.862	24.890	1.00	32.28
ATOM	2756	CD2	HIS	541	68.127	-2.482	26.093	1.00	32.39
ATOM	2757	ND1	HIS	541	67.086	-2.411	24.177	1.00	30.10
ATOM	2758	CE1	HIS	541	66.489	-3.329	24.911	1.00	33.35
ATOM	2759	NE2	HIS	541	67.096	-3.384	26.081	1.00	30.46
ATOM	2760	C	HIS	541	69.720	-2.206	22.275	1.00	35.33
ATOM	2761	O	HIS	541	69.648	-1.614	21.200	1.00	34.87
ATOM	2762	N	LYS	542	69.348	-3.478	22.430	1.00	35.42
ATOM	2763	CA	LYS	542	68.908	-4.311	21.306	1.00	32.02
ATOM	2764	CB	LYS	542	68.715	-5.766	21.753	1.00	30.96
ATOM	2765	C	LYS	542	67.652	-3.848	20.614	1.00	30.02
ATOM	2766	O	LYS	542	67.474	-4.058	19.417	1.00	29.10
ATOM	2767	N	ASN	543	66.778	-3.212	21.369	1.00	28.54
ATOM	2768	CA	ASN	543	65.529	-2.754	20.803	1.00	28.20
ATOM	2769	CB	ASN	543	64.372	-3.241	21.660	1.00	29.73
ATOM	2770	CG	ASN	543	64.387	-4.739	21.840	1.00	30.74
ATOM	2771	OD1	ASN	543	64.732	-5.242	22.909	1.00	32.96
ATOM	2772	ND2	ASN	543	64.053	-5.462	20.787	1.00	29.58
ATOM	2773	C	ASN	543	65.426	-1.257	20.529	1.00	28.06
ATOM	2774	O	ASN	543	64.342	-0.679	20.647	1.00	28.86
ATOM	2775	N	ILE	544	66.546	-0.635	20.168	1.00	26.70
ATOM	2776	CA	ILE	544	66.582	0.794	19.833	1.00	26.81
ATOM	2777	CB	ILE	544	67.052	1.721	21.019	1.00	24.75
ATOM	2778	CG2	ILE	544	66.338	1.353	22.306	1.00	20.02
ATOM	2779	CG1	ILE	544	68.568	1.614	21.234	1.00	23.73
ATOM	2780	CD1	ILE	544	69.105	2.531	22.332	1.00	21.64
ATOM	2781	C	ILE	544	67.582	0.901	18.680	1.00	27.95
ATOM	2782	O	ILE	544	68.388	-0.008	18.480	1.00	26.80
ATOM	2783	N	ILE	545	67.449	1.940	17.849	1.00	29.22
ATOM	2784	CA	ILE	545	68.376	2.163	16.745	1.00	27.14
ATOM	2785	CB	ILE	545	67.824	3.164	15.709	1.00	26.10
ATOM	2786	CG2	ILE	545	68.920	3.556	14.731	1.00	24.70
ATOM	2787	CG1	ILE	545	66.625	2.568	14.955	1.00	23.78
ATOM	2788	CD1	ILE	545	66.988	1.326	14.117	1.00	22.15
ATOM	2789	C	ILE	545	69.631	2.718	17.401	1.00	28.14
ATOM	2790	O	ILE	545	69.586	3.752	18.068	1.00	28.21
ATOM	2791	N	ASN	546	70.740	2.011	17.221	1.00	28.40
ATOM	2792	CA	ASN	546	72.004	2.382	17.822	1.00	28.49
ATOM	2793	CB	ASN	546	72.709	1.122	18.345	1.00	27.05
ATOM	2794	CG	ASN	546	71.956	0.463	19.470	1.00	27.29
ATOM	2795	OD1	ASN	546	71.793	1.031	20.540	1.00	29.92
ATOM	2796	ND2	ASN	546	71.472	-0.740	19.235	1.00	24.63
ATOM	2797	C	ASN	546	72.982	3.124	16.941	1.00	28.39
ATOM	2798	O	ASN	546	73.045	2.894	15.732	1.00	29.62
ATOM	2799	N	LEU	547	73.774	3.982	17.579	1.00	29.91
ATOM	2800	CA	LEU	547	74.828	4.750	16.925	1.00	30.68
ATOM	2801	CB	LEU	547	75.297	5.898	17.837	1.00	25.28
ATOM	2802	CG	LEU	547	76.367	6.828	17.267	1.00	24.81

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ATOM	2803	CD1	LEU	547	75.868	7.524	15.990	1.00	22.25
ATOM	2804	CD2	LEU	547	76.716	7.853	18.313	1.00	24.17
ATOM	2805	C	LEU	547	76.016	3.812	16.629	1.00	31.67
ATOM	2806	O	LEU	547	76.481	3.090	17.509	1.00	31.34
ATOM	2807	N	LEU	548	76.475	3.823	15.380	1.00	30.60
ATOM	2808	CA	LEU	548	77.594	2.995	14.955	1.00	29.31
ATOM	2809	CB	LEU	548	77.197	2.165	13.729	1.00	25.94
ATOM	2810	CG	LEU	548	75.968	1.247	13.883	1.00	28.78
ATOM	2811	CD1	LEU	548	75.848	0.360	12.659	1.00	27.14
ATOM	2812	CD2	LEU	548	76.049	0.392	15.149	1.00	23.72
ATOM	2813	C	LEU	548	78.850	3.821	14.644	1.00	31.60
ATOM	2814	O	LEU	548	79.967	3.330	14.753	1.00	32.65
ATOM	2815	N	GLY	549	78.665	5.076	14.248	1.00	32.22
ATOM	2816	CA	GLY	549	79.795	5.928	13.937	1.00	31.40
ATOM	2817	C	GLY	549	79.344	7.267	13.391	1.00	30.78
ATOM	2818	O	GLY	549	78.140	7.536	13.291	1.00	29.84
ATOM	2819	N	ALA	550	80.320	8.099	13.045	1.00	31.88
ATOM	2820	CA	ALA	550	80.073	9.416	12.485	1.00	30.14
ATOM	2821	CB	ALA	550	79.634	10.382	13.590	1.00	31.08
ATOM	2822	C	ALA	550	81.291	9.978	11.742	1.00	28.78
ATOM	2823	O	ALA	550	82.447	9.705	12.102	1.00	26.39
ATOM	2824	N	CYS	551	81.011	10.690	10.651	1.00	28.48
ATOM	2825	CA	CYS	551	82.012	11.391	9.846	1.00	23.69
ATOM	2826	CB	CYS	551	81.825	11.128	8.352	1.00	24.18
ATOM	2827	SG	CYS	551	81.870	9.395	7.840	1.00	28.40
ATOM	2828	C	CYS	551	81.612	12.847	10.127	1.00	20.99
ATOM	2829	O	CYS	551	80.561	13.282	9.684	1.00	22.11
ATOM	2830	N	THR	552	82.357	13.524	10.996	1.00	20.18
ATOM	2831	CA	THR	552	82.073	14.914	11.349	1.00	22.79
ATOM	2832	CB	THR	552	82.090	15.080	12.874	1.00	23.16
ATOM	2833	OG1	THR	552	83.408	14.803	13.363	1.00	23.52
ATOM	2834	CG2	THR	552	81.125	14.112	13.529	1.00	25.31
ATOM	2835	C	THR	552	83.138	15.886	10.824	1.00	24.74
ATOM	2836	O	THR	552	82.939	17.103	10.782	1.00	22.75
ATOM	2837	N	GLN	553	84.276	15.334	10.431	1.00	26.82
ATOM	2838	CA	GLN	553	85.387	16.153	9.980	1.00	26.99
ATOM	2839	CB	GLN	553	86.686	15.627	10.602	1.00	26.40
ATOM	2840	CG	GLN	553	86.632	15.494	12.141	1.00	22.69
ATOM	2841	CD	GLN	553	86.438	16.836	12.823	1.00	25.90
ATOM	2842	OE1	GLN	553	87.259	17.729	12.656	1.00	29.03
ATOM	2843	NE2	GLN	553	85.351	16.994	13.566	1.00	23.53
ATOM	2844	C	GLN	553	85.502	16.216	8.466	1.00	26.23
ATOM	2845	O	GLN	553	85.177	15.259	7.779	1.00	30.00
ATOM	2846	N	ASP	554	85.863	17.394	7.968	1.00	26.54
ATOM	2847	CA	ASP	554	86.084	17.631	6.531	1.00	28.38
ATOM	2848	CB	ASP	554	87.410	17.031	6.105	1.00	26.78
ATOM	2849	CG	ASP	554	88.538	17.570	6.912	1.00	31.53
ATOM	2850	OD1	ASP	554	88.789	18.795	6.823	1.00	35.18
ATOM	2851	OD2	ASP	554	89.141	16.795	7.665	1.00	29.04
ATOM	2852	C	ASP	554	85.011	17.221	5.545	1.00	29.14
ATOM	2853	O	ASP	554	85.278	16.468	4.610	1.00	31.22
ATOM	2854	N	GLY	555	83.824	17.793	5.709	1.00	31.20

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ATOM	2855	CA	GLY	555	82.723	17.490	4.811	1.00	28.83
ATOM	2856	C	GLY	555	81.446	17.413	5.602	1.00	24.84
ATOM	2857	O	GLY	555	81.448	17.647	6.814	1.00	21.78
ATOM	2858	N	PRO	556	80.317	17.093	4.953	1.00	24.29
ATOM	2859	CD	PRO	556	80.213	16.781	3.510	1.00	19.37
ATOM	2860	CA	PRO	556	79.010	16.973	5.615	1.00	25.11
ATOM	2861	CB	PRO	556	78.107	16.497	4.477	1.00	22.88
ATOM	2862	CG	PRO	556	79.077	15.832	3.485	1.00	23.50
ATOM	2863	C	PRO	556	79.006	15.982	6.777	1.00	27.67
ATOM	2864	O	PRO	556	79.676	14.947	6.736	1.00	27.13
ATOM	2865	N	LEU	557	78.253	16.297	7.820	1.00	29.27
ATOM	2866	CA	LEU	557	78.164	15.405	8.972	1.00	31.19
ATOM	2867	CB	LEU	557	77.583	16.130	10.188	1.00	29.94
ATOM	2868	CG	LEU	557	77.019	15.260	11.323	1.00	26.87
ATOM	2869	CD1	LEU	557	78.131	14.540	12.062	1.00	23.83
ATOM	2870	CD2	LEU	557	76.237	16.146	12.275	1.00	23.80
ATOM	2871	C	LEU	557	77.291	14.193	8.651	1.00	31.97
ATOM	2872	O	LEU	557	76.158	14.332	8.184	1.00	31.18
ATOM	2873	N	TYR	558	77.857	13.010	8.882	1.00	31.12
ATOM	2874	CA	TYR	558	77.145	11.767	8.664	1.00	28.86
ATOM	2875	CB	TYR	558	77.905	10.869	7.694	1.00	28.58
ATOM	2876	CG	TYR	558	78.017	11.395	6.281	1.00	32.33
ATOM	2877	CD1	TYR	558	79.034	10.962	5.443	1.00	35.23
ATOM	2878	CE1	TYR	558	79.161	11.447	4.151	1.00	37.54
ATOM	2879	CD2	TYR	558	77.123	12.336	5.787	1.00	35.27
ATOM	2880	CE2	TYR	558	77.248	12.832	4.493	1.00	36.43
ATOM	2881	CZ	TYR	558	78.276	12.382	3.680	1.00	37.05
ATOM	2882	OH	TYR	558	78.423	12.869	2.394	1.00	39.97
ATOM	2883	C	TYR	558	77.000	11.071	10.004	1.00	26.63
ATOM	2884	O	TYR	558	77.985	10.885	10.725	1.00	24.67
ATOM	2885	N	VAL	559	75.756	10.774	10.365	1.00	28.15
ATOM	2886	CA	VAL	559	75.429	10.070	11.610	1.00	27.70
ATOM	2887	CB	VAL	559	74.262	10.770	12.372	1.00	26.63
ATOM	2888	CG1	VAL	559	73.876	9.959	13.603	1.00	24.70
ATOM	2889	CG2	VAL	559	74.673	12.186	12.792	1.00	26.71
ATOM	2890	C	VAL	559	75.061	8.635	11.205	1.00	27.08
ATOM	2891	O	VAL	559	73.965	8.357	10.710	1.00	25.39
ATOM	2892	N	ILE	560	76.002	7.729	11.399	1.00	28.25
ATOM	2893	CA	ILE	560	75.820	6.335	11.000	1.00	29.62
ATOM	2894	CB	ILE	560	77.225	5.682	10.678	1.00	30.06
ATOM	2895	CG2	ILE	560	77.045	4.279	10.101	1.00	31.58
ATOM	2896	CG1	ILE	560	78.004	6.557	9.686	1.00	27.50
ATOM	2897	CD1	ILE	560	79.492	6.239	9.629	1.00	23.31
ATOM	2898	C	ILE	560	75.075	5.488	12.032	1.00	29.88
ATOM	2899	O	ILE	560	75.586	5.234	13.130	1.00	27.32
ATOM	2900	N	VAL	561	73.857	5.078	11.687	1.00	29.09
ATOM	2901	CA	VAL	561	73.053	4.228	12.568	1.00	28.70
ATOM	2902	CB	VAL	561	71.743	4.932	13.037	1.00	25.29
ATOM	2903	CG1	VAL	561	72.072	6.139	13.872	1.00	22.91
ATOM	2904	CG2	VAL	561	70.887	5.312	11.870	1.00	22.38
ATOM	2905	C	VAL	561	72.731	2.848	11.945	1.00	27.99
ATOM	2906	O	VAL	561	73.052	2.590	10.783	1.00	27.88

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ATOM	2907	N	GLU	562	72.143	1.969	12.754	1.00	27.38
ATOM	2908	CA	GLU	562	71.759	0.616	12.347	1.00	28.01
ATOM	2909	CB	GLU	562	71.246	-0.161	13.555	1.00	25.37
ATOM	2910	CG	GLU	562	72.322	-0.487	14.570	1.00	29.22
ATOM	2911	CD	GLU	562	71.785	-1.190	15.796	1.00	30.94
ATOM	2912	OE1	GLU	562	72.440	-2.135	16.271	1.00	34.82
ATOM	2913	OE2	GLU	562	70.716	-0.795	16.297	1.00	32.77
ATOM	2914	C	GLU	562	70.695	0.610	11.266	1.00	29.83
ATOM	2915	O	GLU	562	69.822	1.452	11.274	1.00	34.69
ATOM	2916	N	TYR	563	70.755	-0.364	10.362	1.00	31.35
ATOM	2917	CA	TYR	563	69.806	-0.527	9.255	1.00	33.79
ATOM	2918	CB	TYR	563	70.586	-0.987	8.022	1.00	32.37
ATOM	2919	CG	TYR	563	69.759	-1.232	6.778	1.00	31.70
ATOM	2920	CD1	TYR	563	68.858	-0.277	6.319	1.00	35.00
ATOM	2921	CE1	TYR	563	68.101	-0.490	5.161	1.00	35.62
ATOM	2922	CD2	TYR	563	69.888	-2.416	6.053	1.00	31.64
ATOM	2923	CE2	TYR	563	69.138	-2.644	4.894	1.00	32.96
ATOM	2924	CZ	TYR	563	68.242	-1.674	4.462	1.00	36.20
ATOM	2925	OH	TYR	563	67.494	-1.906	3.340	1.00	39.54
ATOM	2926	C	TYR	563	68.668	-1.527	9.593	1.00	37.26
ATOM	2927	O	TYR	563	68.915	-2.566	10.212	1.00	38.86
ATOM	2928	N	ALA	564	67.428	-1.180	9.220	1.00	39.09
ATOM	2929	CA	ALA	564	66.256	-2.027	9.467	1.00	37.64
ATOM	2930	CB	ALA	564	65.290	-1.317	10.366	1.00	41.34
ATOM	2931	C	ALA	564	65.600	-2.337	8.124	1.00	39.33
ATOM	2932	O	ALA	564	64.700	-1.628	7.661	1.00	41.28
ATOM	2933	N	SER	565	66.033	-3.432	7.515	1.00	40.21
ATOM	2934	CA	SER	565	65.567	-3.867	6.202	1.00	40.22
ATOM	2935	CB	SER	565	66.302	-5.133	5.808	1.00	38.50
ATOM	2936	OG	SER	565	66.174	-6.084	6.847	1.00	37.66
ATOM	2937	C	SER	565	64.095	-4.087	5.987	1.00	42.30
ATOM	2938	O	SER	565	63.657	-4.155	4.840	1.00	46.83
ATOM	2939	N	LYS	566	63.322	-4.248	7.054	1.00	42.84
ATOM	2940	CA	LYS	566	61.893	-4.462	6.883	1.00	41.84
ATOM	2941	CB	LYS	566	61.455	-5.681	7.684	1.00	44.88
ATOM	2942	CG	LYS	566	62.003	-6.977	7.088	1.00	48.86
ATOM	2943	CD	LYS	566	61.929	-8.148	8.040	1.00	51.41
ATOM	2944	CE	LYS	566	62.582	-9.362	7.426	1.00	53.89
ATOM	2945	NZ	LYS	566	62.706	-10.465	8.417	1.00	59.37
ATOM	2946	C	LYS	566	61.029	-3.234	7.143	1.00	41.89
ATOM	2947	O	LYS	566	59.815	-3.337	7.341	1.00	43.68
ATOM	2948	N	GLY	567	61.663	-2.061	7.100	1.00	39.50
ATOM	2949	CA	GLY	567	60.956	-0.808	7.291	1.00	36.69
ATOM	2950	C	GLY	567	60.306	-0.640	8.644	1.00	35.86
ATOM	2951	O	GLY	567	60.727	-1.265	9.614	1.00	35.90
ATOM	2952	N	ASN	568	59.296	0.218	8.711	1.00	35.45
ATOM	2953	CA	ASN	568	58.615	0.447	9.966	1.00	38.10
ATOM	2954	CB	ASN	568	57.961	1.839	10.029	1.00	40.77
ATOM	2955	CG	ASN	568	56.701	1.962	9.163	1.00	43.52
ATOM	2956	OD1	ASN	568	55.718	1.241	9.338	1.00	44.01
ATOM	2957	ND2	ASN	568	56.710	2.932	8.263	1.00	45.39
ATOM	2958	C	ASN	568	57.610	-0.657	10.269	1.00	38.91

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ATOM	2959	O	ASN	568	57.218	-1.420	9.384	1.00	39.95
ATOM	2960	N	LEU	569	57.204	-0.717	11.534	1.00	38.93
ATOM	2961	CA	LEU	569	56.256	-1.692	12.047	1.00	36.49
ATOM	2962	CB	LEU	569	56.126	-1.507	13.555	1.00	36.53
ATOM	2963	CG	LEU	569	55.150	-2.417	14.290	1.00	35.27
ATOM	2964	CD1	LEU	569	55.550	-3.865	14.047	1.00	31.86
ATOM	2965	CD2	LEU	569	55.148	-2.067	15.768	1.00	35.00
ATOM	2966	C	LEU	569	54.875	-1.622	11.391	1.00	37.19
ATOM	2967	O	LEU	569	54.231	-2.654	11.175	1.00	38.40
ATOM	2968	N	ARG	570	54.386	-0.420	11.101	1.00	36.63
ATOM	2969	CA	ARG	570	53.068	-0.294	10.485	1.00	36.68
ATOM	2970	CB	ARG	570	52.739	1.168	10.188	1.00	37.76
ATOM	2971	CG	ARG	570	51.339	1.361	9.623	1.00	46.41
ATOM	2972	CD	ARG	570	51.210	2.680	8.889	1.00	56.33
ATOM	2973	NE	ARG	570	52.162	2.785	7.779	1.00	63.05
ATOM	2974	CZ	ARG	570	53.010	3.798	7.603	1.00	66.33
ATOM	2975	NH1	ARG	570	53.032	4.809	8.468	1.00	65.15
ATOM	2976	NH2	ARG	570	53.853	3.786	6.580	1.00	66.56
ATOM	2977	C	ARG	570	53.046	-1.094	9.193	1.00	35.55
ATOM	2978	O	ARG	570	52.248	-2.015	9.018	1.00	35.33
ATOM	2979	N	GLU	571	53.978	-0.758	8.320	1.00	37.20
ATOM	2980	CA	GLU	571	54.128	-1.401	7.030	1.00	38.32
ATOM	2981	CB	GLU	571	55.247	-0.695	6.261	1.00	40.15
ATOM	2982	CG	GLU	571	55.001	0.803	6.152	1.00	49.09
ATOM	2983	CD	GLU	571	56.118	1.557	5.442	1.00	58.16
ATOM	2984	OE1	GLU	571	57.279	1.073	5.421	1.00	61.41
ATOM	2985	OE2	GLU	571	55.824	2.660	4.914	1.00	61.27
ATOM	2986	C	GLU	571	54.406	-2.906	7.170	1.00	36.74
ATOM	2987	O	GLU	571	53.863	-3.721	6.410	1.00	35.74
ATOM	2988	N	TYR	572	55.241	-3.266	8.141	1.00	35.13
ATOM	2989	CA	TYR	572	55.591	-4.665	8.401	1.00	37.12
ATOM	2990	CB	TYR	572	56.591	-4.736	9.560	1.00	34.39
ATOM	2991	CG	TYR	572	56.984	-6.128	10.029	1.00	33.48
ATOM	2992	CD1	TYR	572	57.980	-6.869	9.367	1.00	29.76
ATOM	2993	CE1	TYR	572	58.394	-8.119	9.845	1.00	27.14
ATOM	2994	CD2	TYR	572	56.406	-6.681	11.183	1.00	32.40
ATOM	2995	CE2	TYR	572	56.814	-7.931	11.669	1.00	30.83
ATOM	2996	CZ	TYR	572	57.807	-8.641	10.995	1.00	33.73
ATOM	2997	OH	TYR	572	58.201	-9.872	11.480	1.00	37.16
ATOM	2998	C	TYR	572	54.330	-5.468	8.729	1.00	38.92
ATOM	2999	O	TYR	572	54.108	-6.553	8.183	1.00	39.22
ATOM	3000	N	LEU	573	53.507	-4.922	9.618	1.00	38.41
ATOM	3001	CA	LEU	573	52.261	-5.563	10.016	1.00	37.56
ATOM	3002	CB	LEU	573	51.573	-4.711	11.084	1.00	36.44
ATOM	3003	CG	LEU	573	52.270	-4.617	12.437	1.00	33.91
ATOM	3004	CD1	LEU	573	51.555	-3.626	13.372	1.00	31.60
ATOM	3005	CD2	LEU	573	52.313	-6.024	13.003	1.00	30.78
ATOM	3006	C	LEU	573	51.315	-5.738	8.826	1.00	37.51
ATOM	3007	O	LEU	573	50.847	-6.836	8.539	1.00	36.70
ATOM	3008	N	GLN	574	51.045	-4.643	8.125	1.00	40.10
ATOM	3009	CA	GLN	574	50.141	-4.678	6.986	1.00	41.10
ATOM	3010	CB	GLN	574	49.938	-3.272	6.439	1.00	40.12

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ATOM	3011	CG	GLN	574	49.171	-2.381	7.374	1.00	40.77
ATOM	3012	CD	GLN	574	49.079	-0.987	6.852	1.00	43.90
ATOM	3013	OE1	GLN	574	49.679	-0.652	5.835	1.00	46.93
ATOM	3014	NE2	GLN	574	48.357	-0.143	7.558	1.00	46.85
ATOM	3015	C	GLN	574	50.546	-5.638	5.875	1.00	41.31
ATOM	3016	O	GLN	574	49.699	-6.323	5.309	1.00	44.33
ATOM	3017	N	ALA	575	51.840	-5.735	5.601	1.00	41.46
ATOM	3018	CA	ALA	575	52.317	-6.628	4.555	1.00	39.80
ATOM	3019	CB	ALA	575	53.745	-6.301	4.218	1.00	40.58
ATOM	3020	C	ALA	575	52.197	-8.096	4.947	1.00	40.86
ATOM	3021	O	ALA	575	52.527	-8.975	4.165	1.00	41.50
ATOM	3022	N	ARG	576	51.757	-8.359	6.168	1.00	42.47
ATOM	3023	CA	ARG	576	51.624	-9.726	6.641	1.00	42.68
ATOM	3024	CB	ARG	576	52.679	-9.988	7.716	1.00	41.04
ATOM	3025	CG	ARG	576	54.095	-9.958	7.161	1.00	42.73
ATOM	3026	CD	ARG	576	55.156	-9.943	8.257	1.00	45.59
ATOM	3027	NE	ARG	576	56.514	-9.870	7.695	1.00	43.89
ATOM	3028	CZ	ARG	576	56.981	-8.856	6.969	1.00	43.35
ATOM	3029	NH1	ARG	576	56.219	-7.803	6.703	1.00	44.85
ATOM	3030	NH2	ARG	576	58.215	-8.902	6.497	1.00	41.84
ATOM	3031	C	ARG	576	50.232	-10.014	7.180	1.00	44.86
ATOM	3032	O	ARG	576	50.043	-10.943	7.970	1.00	46.08
ATOM	3033	N	ARG	577	49.258	-9.216	6.753	1.00	46.72
ATOM	3034	CA	ARG	577	47.877	-9.401	7.196	1.00	47.61
ATOM	3035	CB	ARG	577	46.994	-8.239	6.723	1.00	46.35
ATOM	3036	CG	ARG	577	47.101	-6.995	7.581	1.00	47.71
ATOM	3037	CD	ARG	577	46.329	-5.831	6.999	1.00	49.15
ATOM	3038	NE	ARG	577	46.213	-4.735	7.957	1.00	53.23
ATOM	3039	CZ	ARG	577	45.584	-3.587	7.725	1.00	54.38
ATOM	3040	NH1	ARG	577	45.020	-3.368	6.549	1.00	56.41
ATOM	3041	NH2	ARG	577	45.481	-2.676	8.686	1.00	58.13
ATOM	3042	C	ARG	577	47.298	-10.740	6.743	1.00	47.36
ATOM	3043	O	ARG	577	47.246	-11.031	5.550	1.00	48.52
ATOM	3044	N	GLN	594	53.349	-13.948	7.960	1.00	68.05
ATOM	3045	CA	GLN	594	52.144	-14.067	8.772	1.00	66.75
ATOM	3046	CB	GLN	594	51.259	-15.220	8.277	1.00	66.87
ATOM	3047	C	GLN	594	52.535	-14.284	10.233	1.00	64.71
ATOM	3048	O	GLN	594	53.192	-15.264	10.580	1.00	64.86
ATOM	3049	N	LEU	595	52.159	-13.335	11.074	1.00	61.14
ATOM	3050	CA	LEU	595	52.489	-13.422	12.480	1.00	58.19
ATOM	3051	CB	LEU	595	52.599	-12.008	13.056	1.00	56.33
ATOM	3052	CG	LEU	595	53.532	-11.147	12.203	1.00	57.36
ATOM	3053	CD1	LEU	595	53.375	-9.692	12.533	1.00	59.51
ATOM	3054	CD2	LEU	595	54.967	-11.598	12.382	1.00	56.98
ATOM	3055	C	LEU	595	51.469	-14.237	13.251	1.00	56.25
ATOM	3056	O	LEU	595	50.314	-14.359	12.834	1.00	56.60
ATOM	3057	N	SER	596	51.927	-14.845	14.341	1.00	53.07
ATOM	3058	CA	SER	596	51.100	-15.642	15.229	1.00	48.64
ATOM	3059	CB	SER	596	51.883	-16.841	15.736	1.00	46.41
ATOM	3060	OG	SER	596	52.806	-16.435	16.737	1.00	46.50
ATOM	3061	C	SER	596	50.796	-14.756	16.423	1.00	48.95
ATOM	3062	O	SER	596	51.492	-13.767	16.649	1.00	49.39

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ATOM	3063	N	SER	597	49.833	-15.163	17.242	1.00	50.27
ATOM	3064	CA	SER	597	49.469	-14.387	18.424	1.00	51.93
ATOM	3065	CB	SER	597	48.391	-15.123	19.225	1.00	52.03
ATOM	3066	OG	SER	597	47.540	-15.854	18.365	1.00	52.95
ATOM	3067	C	SER	597	50.685	-14.143	19.314	1.00	52.72
ATOM	3068	O	SER	597	50.792	-13.093	19.943	1.00	55.04
ATOM	3069	N	LYS	598	51.613	-15.100	19.344	1.00	53.55
ATOM	3070	CA	LYS	598	52.824	-14.961	20.159	1.00	53.84
ATOM	3071	CB	LYS	598	53.566	-16.295	20.248	1.00	54.25
ATOM	3072	CG	LYS	598	54.376	-16.457	21.524	1.00	57.30
ATOM	3073	CD	LYS	598	55.057	-17.824	21.570	1.00	58.11
ATOM	3074	CE	LYS	598	55.780	-18.055	22.893	1.00	59.00
ATOM	3075	NZ	LYS	598	54.840	-18.169	24.043	1.00	57.85
ATOM	3076	C	LYS	598	53.728	-13.909	19.527	1.00	52.48
ATOM	3077	O	LYS	598	54.273	-13.052	20.227	1.00	51.72
ATOM	3078	N	ASP	599	53.842	-13.960	18.198	1.00	50.65
ATOM	3079	CA	ASP	599	54.657	-13.021	17.435	1.00	48.52
ATOM	3080	CB	ASP	599	54.568	-13.294	15.929	1.00	46.71
ATOM	3081	CG	ASP	599	55.233	-14.607	15.515	1.00	48.88
ATOM	3082	OD1	ASP	599	55.898	-15.260	16.344	1.00	53.76
ATOM	3083	OD2	ASP	599	55.100	-14.986	14.330	1.00	46.70
ATOM	3084	C	ASP	599	54.173	-11.598	17.706	1.00	48.66
ATOM	3085	O	ASP	599	54.976	-10.703	17.960	1.00	52.86
ATOM	3086	N	LEU	600	52.852	-11.406	17.684	1.00	44.53
ATOM	3087	CA	LEU	600	52.272	-10.099	17.938	1.00	41.06
ATOM	3088	CB	LEU	600	50.774	-10.100	17.632	1.00	39.23
ATOM	3089	CG	LEU	600	50.354	-10.374	16.178	1.00	36.50
ATOM	3090	CD1	LEU	600	48.850	-10.272	16.063	1.00	34.99
ATOM	3091	CD2	LEU	600	51.000	-9.393	15.232	1.00	33.72
ATOM	3092	C	LEU	600	52.543	-9.633	19.369	1.00	40.96
ATOM	3093	O	LEU	600	52.890	-8.467	19.580	1.00	42.04
ATOM	3094	N	VAL	601	52.417	-10.533	20.348	1.00	41.02
ATOM	3095	CA	VAL	601	52.685	-10.156	21.744	1.00	43.57
ATOM	3096	CB	VAL	601	52.236	-11.229	22.791	1.00	43.60
ATOM	3097	CG1	VAL	601	52.254	-10.607	24.205	1.00	43.44
ATOM	3098	CG2	VAL	601	50.848	-11.761	22.464	1.00	42.33
ATOM	3099	C	VAL	601	54.192	-9.904	21.901	1.00	42.85
ATOM	3100	O	VAL	601	54.611	-8.989	22.611	1.00	44.28
ATOM	3101	N	SER	602	54.986	-10.685	21.175	1.00	41.33
ATOM	3102	CA	SER	602	56.442	-10.581	21.180	1.00	41.43
ATOM	3103	CB	SER	602	57.014	-11.648	20.245	1.00	40.94
ATOM	3104	OG	SER	602	58.434	-11.612	20.184	1.00	46.26
ATOM	3105	C	SER	602	56.859	-9.176	20.722	1.00	40.58
ATOM	3106	O	SER	602	57.629	-8.497	21.403	1.00	42.32
ATOM	3107	N	CYS	603	56.318	-8.737	19.589	1.00	38.34
ATOM	3108	CA	CYS	603	56.580	-7.409	19.051	1.00	37.28
ATOM	3109	CB	CYS	603	55.715	-7.170	17.815	1.00	38.09
ATOM	3110	SG	CYS	603	55.735	-5.497	17.170	0.50	42.18
ATOM	3111	C	CYS	603	56.282	-6.337	20.105	1.00	35.81
ATOM	3112	O	CYS	603	57.038	-5.380	20.241	1.00	37.87
ATOM	3113	N	ALA	604	55.198	-6.508	20.858	1.00	33.96
ATOM	3114	CA	ALA	604	54.804	-5.572	21.911	1.00	34.97

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ATOM	3115	CB	ALA	604	53.393	-5.917	22.409	1.00	34.13
ATOM	3116	C	ALA	604	55.791	-5.610	23.081	1.00	36.68
ATOM	3117	O	ALA	604	56.085	-4.585	23.704	1.00	36.78
ATOM	3118	N	TYR	605	56.281	-6.807	23.385	1.00	37.68
ATOM	3119	CA	TYR	605	57.254	-7.005	24.461	1.00	38.38
ATOM	3120	CB	TYR	605	57.533	-8.498	24.643	1.00	37.62
ATOM	3121	CG	TYR	605	58.635	-8.806	25.622	1.00	36.56
ATOM	3122	CD1	TYR	605	58.498	-8.509	26.974	1.00	39.05
ATOM	3123	CE1	TYR	605	59.520	-8.809	27.893	1.00	41.37
ATOM	3124	CD2	TYR	605	59.812	-9.407	25.198	1.00	38.09
ATOM	3125	CE2	TYR	605	60.848	-9.711	26.105	1.00	38.55
ATOM	3126	CZ	TYR	605	60.692	-9.409	27.454	1.00	40.73
ATOM	3127	OH	TYR	605	61.707	-9.704	28.348	1.00	41.44
ATOM	3128	C	TYR	605	58.549	-6.267	24.123	1.00	38.44
ATOM	3129	O	TYR	605	59.053	-5.485	24.937	1.00	40.78
ATOM	3130	N	GLN	606	59.053	-6.501	22.908	1.00	36.07
ATOM	3131	CA	GLN	606	60.276	-5.872	22.398	1.00	35.28
ATOM	3132	CB	GLN	606	60.594	-6.415	21.002	1.00	34.24
ATOM	3133	CG	GLN	606	61.105	-7.851	21.005	1.00	32.26
ATOM	3134	CD	GLN	606	61.339	-8.388	19.608	1.00	30.17
ATOM	3135	OE1	GLN	606	62.274	-7.988	18.907	1.00	31.89
ATOM	3136	NE2	GLN	606	60.471	-9.285	19.182	1.00	30.68
ATOM	3137	C	GLN	606	60.210	-4.335	22.355	1.00	36.39
ATOM	3138	O	GLN	606	61.206	-3.660	22.632	1.00	39.59
ATOM	3139	N	VAL	607	59.040	-3.798	22.006	1.00	32.78
ATOM	3140	CA	VAL	607	58.839	-2.350	21.944	1.00	30.29
ATOM	3141	CB	VAL	607	57.489	-1.982	21.221	1.00	28.48
ATOM	3142	CG1	VAL	607	57.219	-0.488	21.298	1.00	28.68
ATOM	3143	CG2	VAL	607	57.535	-2.416	19.742	1.00	22.96
ATOM	3144	C	VAL	607	58.868	-1.766	23.364	1.00	30.21
ATOM	3145	O	VAL	607	59.469	-0.705	23.591	1.00	31.24
ATOM	3146	N	ALA	608	58.224	-2.451	24.311	1.00	27.88
ATOM	3147	CA	ALA	608	58.187	-2.001	25.694	1.00	27.66
ATOM	3148	CB	ALA	608	57.242	-2.874	26.494	1.00	26.42
ATOM	3149	C	ALA	608	59.585	-2.019	26.309	1.00	29.04
ATOM	3150	O	ALA	608	59.950	-1.144	27.094	1.00	27.53
ATOM	3151	N	ARG	609	60.377	-3.013	25.932	1.00	28.91
ATOM	3152	CA	ARG	609	61.733	-3.120	26.440	1.00	31.64
ATOM	3153	CB	ARG	609	62.394	-4.405	25.953	1.00	33.78
ATOM	3154	CG	ARG	609	61.672	-5.647	26.373	1.00	38.53
ATOM	3155	CD	ARG	609	62.636	-6.791	26.448	1.00	41.78
ATOM	3156	NE	ARG	609	63.319	-6.838	27.733	1.00	47.58
ATOM	3157	CZ	ARG	609	64.441	-7.510	27.955	1.00	51.52
ATOM	3158	NH1	ARG	609	65.012	-8.179	26.964	1.00	50.61
ATOM	3159	NH2	ARG	609	64.954	-7.569	29.186	1.00	54.36
ATOM	3160	C	ARG	609	62.581	-1.918	26.024	1.00	33.26
ATOM	3161	O	ARG	609	63.144	-1.221	26.885	1.00	34.50
ATOM	3162	N	GLY	610	62.624	-1.650	24.717	1.00	30.25
ATOM	3163	CA	GLY	610	63.395	-0.534	24.199	1.00	25.40
ATOM	3164	C	GLY	610	63.010	0.730	24.930	1.00	24.12
ATOM	3165	O	GLY	610	63.857	1.507	25.345	1.00	24.74
ATOM	3166	N	MET	611	61.712	0.907	25.131	1.00	25.81

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ATOM	3167	CA	MET	611	61.192	2.062	25.843	1.00	26.95
ATOM	3168	CB	MET	611	59.672	2.121	25.702	1.00	24.60
ATOM	3169	CG	MET	611	59.215	2.462	24.303	1.00	24.10
ATOM	3170	SD	MET	611	59.972	4.035	23.821	1.00	26.77
ATOM	3171	CE	MET	611	59.546	5.090	25.184	1.00	19.21
ATOM	3172	C	MET	611	61.600	2.071	27.314	1.00	27.68
ATOM	3173	O	MET	611	61.891	3.128	27.865	1.00	28.22
ATOM	3174	N	GLU	612	61.562	0.908	27.967	1.00	31.07
ATOM	3175	CA	GLU	612	61.955	0.791	29.382	1.00	35.25
ATOM	3176	CB	GLU	612	61.809	-0.659	29.872	1.00	34.95
ATOM	3177	CG	GLU	612	62.383	-0.937	31.257	1.00	31.64
ATOM	3178	CD	GLU	612	62.392	-2.422	31.631	1.00	32.34
ATOM	3179	OE1	GLU	612	62.599	-3.275	30.738	1.00	30.09
ATOM	3180	OE2	GLU	612	62.226	-2.737	32.831	1.00	33.90
ATOM	3181	C	GLU	612	63.409	1.252	29.468	1.00	37.14
ATOM	3182	O	GLU	612	63.791	1.995	30.390	1.00	35.60
ATOM	3183	N	TYR	613	64.196	0.868	28.457	1.00	37.89
ATOM	3184	CA	TYR	613	65.601	1.247	28.392	1.00	36.68
ATOM	3185	CB	TYR	613	66.328	0.531	27.246	1.00	34.23
ATOM	3186	CG	TYR	613	67.801	0.888	27.175	1.00	36.59
ATOM	3187	CD1	TYR	613	68.734	0.263	28.005	1.00	36.83
ATOM	3188	CE1	TYR	613	70.090	0.649	28.013	1.00	34.51
ATOM	3189	CD2	TYR	613	68.252	1.909	26.339	1.00	35.28
ATOM	3190	CE2	TYR	613	69.596	2.306	26.340	1.00	34.09
ATOM	3191	CZ	TYR	613	70.512	1.674	27.181	1.00	35.91
ATOM	3192	OH	TYR	613	71.826	2.089	27.212	1.00	29.78
ATOM	3193	C	TYR	613	65.724	2.760	28.233	1.00	37.58
ATOM	3194	O	TYR	613	66.362	3.414	29.056	1.00	39.84
ATOM	3195	N	LEU	614	65.081	3.326	27.214	1.00	35.53
ATOM	3196	CA	LEU	614	65.156	4.766	26.988	1.00	34.58
ATOM	3197	CB	LEU	614	64.314	5.157	25.781	1.00	31.88
ATOM	3198	CG	LEU	614	64.760	4.601	24.429	1.00	29.62
ATOM	3199	CD1	LEU	614	63.783	5.016	23.346	1.00	29.19
ATOM	3200	CD2	LEU	614	66.134	5.133	24.111	1.00	32.49
ATOM	3201	C	LEU	614	64.698	5.538	28.218	1.00	36.38
ATOM	3202	O	LEU	614	65.325	6.525	28.618	1.00	33.81
ATOM	3203	N	ALA	615	63.608	5.076	28.821	1.00	38.08
ATOM	3204	CA	ALA	615	63.066	5.711	30.018	1.00	41.01
ATOM	3205	CB	ALA	615	61.767	5.018	30.444	1.00	42.33
ATOM	3206	C	ALA	615	64.099	5.683	31.147	1.00	40.47
ATOM	3207	O	ALA	615	64.291	6.690	31.831	1.00	41.28
ATOM	3208	N	SER	616	64.788	4.553	31.307	1.00	38.78
ATOM	3209	CA	SER	616	65.806	4.441	32.347	1.00	40.97
ATOM	3210	CB	SER	616	66.354	3.009	32.454	1.00	37.82
ATOM	3211	OG	SER	616	67.172	2.651	31.359	1.00	34.73
ATOM	3212	C	SER	616	66.941	5.416	32.061	1.00	42.68
ATOM	3213	O	SER	616	67.714	5.769	32.957	1.00	45.78
ATOM	3214	N	LYS	617	67.015	5.869	30.815	1.00	40.92
ATOM	3215	CA	LYS	617	68.025	6.816	30.380	1.00	38.04
ATOM	3216	CB	LYS	617	68.541	6.411	29.003	1.00	38.25
ATOM	3217	CG	LYS	617	69.293	5.111	29.021	1.00	36.40
ATOM	3218	CD	LYS	617	70.421	5.221	29.992	1.00	38.14

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ATOM	3219	CE	LYS	617	71.215	3.941	30.086	1.00	38.43
ATOM	3220	NZ	LYS	617	72.530	4.210	30.751	1.00	43.07
ATOM	3221	C	LYS	617	67.475	8.242	30.350	1.00	38.42
ATOM	3222	O	LYS	617	68.072	9.133	29.744	1.00	41.37
ATOM	3223	N	LYS	618	66.323	8.444	30.985	1.00	37.25
ATOM	3224	CA	LYS	618	65.674	9.743	31.067	1.00	36.75
ATOM	3225	CB	LYS	618	66.653	10.780	31.632	1.00	43.27
ATOM	3226	CG	LYS	618	67.340	10.392	32.938	1.00	51.59
ATOM	3227	CD	LYS	618	66.377	10.361	34.092	1.00	61.24
ATOM	3228	CE	LYS	618	67.070	9.945	35.373	1.00	67.83
ATOM	3229	NZ	LYS	618	66.105	10.039	36.510	1.00	75.22
ATOM	3230	C	LYS	618	65.167	10.222	29.706	1.00	36.61
ATOM	3231	O	LYS	618	64.856	11.396	29.535	1.00	35.94
ATOM	3232	N	CYS	619	65.058	9.308	28.751	1.00	36.26
ATOM	3233	CA	CYS	619	64.603	9.666	27.412	1.00	33.41
ATOM	3234	CB	CYS	619	65.351	8.843	26.365	1.00	32.17
ATOM	3235	SG	CYS	619	65.006	9.223	24.650	1.00	26.92
ATOM	3236	C	CYS	619	63.108	9.546	27.194	1.00	32.29
ATOM	3237	O	CYS	619	62.510	8.472	27.373	1.00	29.13
ATOM	3238	N	ILE	620	62.515	10.679	26.827	1.00	31.60
ATOM	3239	CA	ILE	620	61.091	10.763	26.528	1.00	31.21
ATOM	3240	CB	ILE	620	60.435	11.966	27.212	1.00	29.57
ATOM	3241	CG2	ILE	620	58.955	12.031	26.860	1.00	31.49
ATOM	3242	CG1	ILE	620	60.578	11.848	28.727	1.00	27.85
ATOM	3243	CD1	ILE	620	60.065	13.046	29.463	1.00	26.50
ATOM	3244	C	ILE	620	61.034	10.972	25.018	1.00	32.18
ATOM	3245	O	ILE	620	61.481	11.993	24.512	1.00	33.18
ATOM	3246	N	HIS	621	60.472	9.990	24.318	1.00	31.93
ATOM	3247	CA	HIS	621	60.354	9.970	22.864	1.00	32.59
ATOM	3248	CB	HIS	621	59.933	8.552	22.420	1.00	29.51
ATOM	3249	CG	HIS	621	60.076	8.288	20.951	1.00	27.45
ATOM	3250	CD2	HIS	621	60.663	7.262	20.286	1.00	25.84
ATOM	3251	ND1	HIS	621	59.528	9.106	19.979	1.00	25.20
ATOM	3252	CE1	HIS	621	59.774	8.596	18.783	1.00	25.07
ATOM	3253	NE2	HIS	621	60.456	7.473	18.942	1.00	23.24
ATOM	3254	C	HIS	621	59.365	10.992	22.320	1.00	35.31
ATOM	3255	O	HIS	621	59.555	11.481	21.220	1.00	39.24
ATOM	3256	N	ARG	622	58.256	11.216	23.028	1.00	36.50
ATOM	3257	CA	ARG	622	57.225	12.169	22.580	1.00	35.78
ATOM	3258	CB	ARG	622	57.783	13.582	22.462	1.00	32.55
ATOM	3259	CG	ARG	622	58.211	14.156	23.778	1.00	30.54
ATOM	3260	CD	ARG	622	58.799	15.551	23.635	0.50	27.28
ATOM	3261	NE	ARG	622	59.249	16.043	24.930	0.50	24.53
ATOM	3262	CZ	ARG	622	60.409	15.707	25.499	0.50	27.85
ATOM	3263	NH1	ARG	622	61.249	14.883	24.877	0.50	27.61
ATOM	3264	NH2	ARG	622	60.711	16.158	26.714	0.50	25.34
ATOM	3265	C	ARG	622	56.447	11.806	21.297	1.00	35.76
ATOM	3266	O	ARG	622	55.438	12.430	20.999	1.00	36.61
ATOM	3267	N	ASP	623	56.923	10.818	20.537	1.00	34.69
ATOM	3268	CA	ASP	623	56.197	10.400	19.335	1.00	34.09
ATOM	3269	CB	ASP	623	56.628	11.171	18.081	1.00	34.77
ATOM	3270	CG	ASP	623	55.727	10.869	16.863	1.00	43.51

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ATOM	3271	OD1	ASP	623	56.213	10.992	15.714	1.00	47.45
ATOM	3272	OD2	ASP	623	54.538	10.509	17.032	1.00	47.51
ATOM	3273	C	ASP	623	56.321	8.903	19.115	1.00	32.51
ATOM	3274	O	ASP	623	56.635	8.435	18.025	1.00	31.80
ATOM	3275	N	LEU	624	56.081	8.135	20.164	1.00	31.80
ATOM	3276	CA	LEU	624	56.152	6.689	20.030	1.00	31.07
ATOM	3277	CB	LEU	624	56.133	6.029	21.403	1.00	28.11
ATOM	3278	CG	LEU	624	55.983	4.510	21.460	1.00	27.88
ATOM	3279	CD1	LEU	624	57.108	3.809	20.700	1.00	23.96
ATOM	3280	CD2	LEU	624	56.001	4.088	22.912	1.00	29.50
ATOM	3281	C	LEU	624	54.954	6.238	19.187	1.00	32.04
ATOM	3282	O	LEU	624	53.805	6.564	19.505	1.00	36.02
ATOM	3283	N	ALA	625	55.224	5.561	18.076	1.00	28.91
ATOM	3284	CA	ALA	625	54.170	5.066	17.192	1.00	25.66
ATOM	3285	CB	ALA	625	53.707	6.170	16.289	1.00	23.37
ATOM	3286	C	ALA	625	54.800	3.948	16.389	1.00	27.71
ATOM	3287	O	ALA	625	56.022	3.841	16.355	1.00	29.77
ATOM	3288	N	ALA	626	53.982	3.107	15.758	1.00	29.46
ATOM	3289	CA	ALA	626	54.499	1.993	14.956	1.00	28.16
ATOM	3290	CB	ALA	626	53.350	1.155	14.401	1.00	28.02
ATOM	3291	C	ALA	626	55.366	2.504	13.831	1.00	26.78
ATOM	3292	O	ALA	626	56.329	1.859	13.454	1.00	26.69
ATOM	3293	N	ARG	627	55.022	3.680	13.314	1.00	26.09
ATOM	3294	CA	ARG	627	55.777	4.301	12.246	1.00	26.78
ATOM	3295	CB	ARG	627	55.134	5.637	11.837	1.00	27.01
ATOM	3296	CG	ARG	627	55.046	6.672	12.961	1.00	29.34
ATOM	3297	CD	ARG	627	54.552	8.037	12.477	1.00	34.26
ATOM	3298	NE	ARG	627	54.108	8.878	13.590	1.00	36.96
ATOM	3299	CZ	ARG	627	52.867	8.889	14.059	1.00	40.84
ATOM	3300	NH1	ARG	627	51.942	8.114	13.515	1.00	42.56
ATOM	3301	NH2	ARG	627	52.552	9.634	15.108	1.00	45.20
ATOM	3302	C	ARG	627	57.209	4.549	12.711	1.00	29.11
ATOM	3303	O	ARG	627	58.137	4.468	11.911	1.00	30.39
ATOM	3304	N	ASN	628	57.385	4.804	14.010	1.00	30.37
ATOM	3305	CA	ASN	628	58.689	5.092	14.596	1.00	27.02
ATOM	3306	CB	ASN	628	58.578	6.226	15.611	1.00	24.35
ATOM	3307	CG	ASN	628	58.383	7.571	14.941	1.00	25.95
ATOM	3308	OD1	ASN	628	58.992	7.865	13.924	1.00	32.01
ATOM	3309	ND2	ASN	628	57.522	8.391	15.503	1.00	24.34
ATOM	3310	C	ASN	628	59.437	3.903	15.185	1.00	26.74
ATOM	3311	O	ASN	628	60.378	4.062	15.972	1.00	28.49
ATOM	3312	N	VAL	629	58.998	2.712	14.802	1.00	27.34
ATOM	3313	CA	VAL	629	59.621	1.450	15.224	1.00	24.94
ATOM	3314	CB	VAL	629	58.589	0.522	15.906	1.00	22.20
ATOM	3315	CG1	VAL	629	59.169	-0.883	16.089	1.00	18.03
ATOM	3316	CG2	VAL	629	58.158	1.121	17.244	1.00	18.34
ATOM	3317	C	VAL	629	60.077	0.805	13.918	1.00	26.84
ATOM	3318	O	VAL	629	59.284	0.679	12.978	1.00	26.50
ATOM	3319	N	LEU	630	61.352	0.469	13.809	1.00	27.66
ATOM	3320	CA	LEU	630	61.862	-0.158	12.601	1.00	30.14
ATOM	3321	CB	LEU	630	63.105	0.577	12.122	1.00	28.00
ATOM	3322	CG	LEU	630	62.856	2.086	12.027	1.00	26.06

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ATOM	3323	CD1	LEU	630	64.150	2.831	11.832	1.00	23.44
ATOM	3324	CD2	LEU	630	61.880	2.381	10.901	1.00	27.72
ATOM	3325	C	LEU	630	62.145	-1.627	12.889	1.00	32.90
ATOM	3326	O	LEU	630	62.437	-1.982	14.029	1.00	33.06
ATOM	3327	N	VAL	631	61.991	-2.478	11.873	1.00	34.83
ATOM	3328	CA	VAL	631	62.195	-3.928	12.006	1.00	33.02
ATOM	3329	CB	VAL	631	60.915	-4.700	11.584	1.00	30.92
ATOM	3330	CG1	VAL	631	61.071	-6.208	11.842	1.00	27.66
ATOM	3331	CG2	VAL	631	59.724	-4.161	12.332	1.00	24.46
ATOM	3332	C	VAL	631	63.371	-4.415	11.161	1.00	35.77
ATOM	3333	O	VAL	631	63.428	-4.171	9.954	1.00	37.57
ATOM	3334	N	THR	632	64.319	-5.098	11.797	1.00	37.96
ATOM	3335	CA	THR	632	65.511	-5.599	11.096	1.00	39.06
ATOM	3336	CB	THR	632	66.675	-5.820	12.066	1.00	35.55
ATOM	3337	OG1	THR	632	66.368	-6.903	12.955	1.00	35.76
ATOM	3338	CG2	THR	632	66.928	-4.561	12.867	1.00	35.06
ATOM	3339	C	THR	632	65.283	-6.893	10.331	1.00	40.66
ATOM	3340	O	THR	632	64.238	-7.515	10.466	1.00	41.79
ATOM	3341	N	GLU	633	66.282	-7.307	9.556	1.00	43.40
ATOM	3342	CA	GLU	633	66.219	-8.540	8.768	1.00	45.33
ATOM	3343	CB	GLU	633	67.501	-8.689	7.942	1.00	48.67
ATOM	3344	CG	GLU	633	67.496	-9.791	6.864	1.00	54.70
ATOM	3345	CD	GLU	633	66.599	-9.506	5.647	1.00	58.16
ATOM	3346	OE1	GLU	633	65.933	-8.452	5.567	1.00	60.68
ATOM	3347	OE2	GLU	633	66.566	-10.369	4.747	1.00	60.14
ATOM	3348	C	GLU	633	66.011	-9.774	9.648	1.00	46.02
ATOM	3349	O	GLU	633	65.637	-10.834	9.156	1.00	46.75
ATOM	3350	N	ASP	634	66.278	-9.648	10.944	1.00	46.45
ATOM	3351	CA	ASP	634	65.085	-10.774	11.843	1.00	46.14
ATOM	3352	CB	ASP	634	67.316	-10.995	12.724	1.00	52.89
ATOM	3353	CG	ASP	634	68.570	-11.399	11.929	1.00	59.65
ATOM	3354	OD1	ASP	634	68.593	-12.499	11.328	1.00	59.91
ATOM	3355	OD2	ASP	634	69.546	-10.608	11.918	1.00	62.29
ATOM	3356	C	ASP	634	64.850	-10.549	12.708	1.00	45.75
ATOM	3357	O	ASP	634	64.729	-11.138	13.776	1.00	46.38
ATOM	3358	N	ASN	635	63.940	-9.697	12.235	1.00	45.92
ATOM	3359	CA	ASN	635	62.690	-9.367	12.915	1.00	44.36
ATOM	3360	CB	ASN	635	61.750	-10.583	12.972	1.00	46.62
ATOM	3361	CG	ASN	635	61.409	-11.116	11.597	1.00	47.56
ATOM	3362	OD1	ASN	635	60.750	-10.453	10.800	1.00	50.54
ATOM	3363	ND2	ASN	635	61.876	-12.314	11.305	1.00	47.75
ATOM	3364	C	ASN	635	62.833	-8.763	14.308	1.00	42.78
ATOM	3365	O	ASN	635	62.028	-9.045	15.189	1.00	44.56
ATOM	3366	N	VAL	636	63.849	-7.927	14.503	1.00	41.03
ATOM	3367	CA	VAL	636	64.071	-7.291	15.797	1.00	36.87
ATOM	3368	CB	VAL	636	65.584	-7.162	16.083	1.00	35.99
ATOM	3369	CG1	VAL	636	65.839	-6.347	17.354	1.00	34.01
ATOM	3370	CG2	VAL	636	66.184	-8.535	16.226	1.00	33.65
ATOM	3371	C	VAL	636	63.434	-5.908	15.782	1.00	34.79
ATOM	3372	O	VAL	636	63.657	-5.131	14.854	1.00	36.58
ATOM	3373	N	MET	637	62.600	-5.625	16.773	1.00	32.04
ATOM	3374	CA	MET	637	61.940	-4.331	16.887	1.00	31.14

ATOM	3375	CB	MET	637	60.734	-4.427	17.817	1.00	35.49
ATOM	3376	CG	MET	637	59.702	-5.501	17.437	1.00	37.77
ATOM	3377	SD	MET	637	58.835	-5.257	15.857	1.00	39.62
ATOM	3378	CE	MET	637	59.122	-6.864	15.035	1.00	34.87
ATOM	3379	C	MET	637	62.935	-3.342	17.479	1.00	29.95
ATOM	3380	O	MET	637	63.525	-3.612	18.526	1.00	26.48
ATOM	3381	N	LYS	638	63.044	-2.167	16.861	1.00	29.03
ATOM	3382	CA	LYS	638	63.977	-1.133	17.293	1.00	24.64
ATOM	3383	CB	LYS	638	65.214	-1.150	16.390	1.00	22.85
ATOM	3384	CG	LYS	638	66.145	-2.305	16.655	1.00	17.56
ATOM	3385	CD	LYS	638	67.307	-2.274	15.707	1.00	19.48
ATOM	3386	CE	LYS	638	68.369	-3.242	16.146	1.00	17.71
ATOM	3387	NZ	LYS	638	68.931	-2.895	17.473	1.00	24.81
ATOM	3388	C	LYS	638	63.367	0.260	17.270	1.00	24.75
ATOM	3389	O	LYS	638	62.987	0.740	16.203	1.00	24.35
ATOM	3390	N	ILE	639	63.277	0.905	18.437	1.00	24.63
ATOM	3391	CA	ILE	639	62.734	2.256	18.536	1.00	24.75
ATOM	3392	CB	ILE	639	62.699	2.789	19.993	1.00	23.98
ATOM	3393	CG2	ILE	639	61.916	4.094	20.046	1.00	21.11
ATOM	3394	CG1	ILE	639	62.127	1.740	20.963	1.00	26.06
ATOM	3395	CD1	ILE	639	60.680	1.392	20.758	1.00	28.45
ATOM	3396	C	ILE	639	63.656	3.198	17.774	1.00	26.36
ATOM	3397	O	ILE	639	64.884	3.161	17.947	1.00	25.06
ATOM	3398	N	ALA	640	63.073	4.072	16.963	1.00	26.70
ATOM	3399	CA	ALA	640	63.857	5.037	16.202	1.00	27.85
ATOM	3400	CB	ALA	640	63.683	4.777	14.736	1.00	27.66
ATOM	3401	C	ALA	640	63.380	6.449	16.548	1.00	29.56
ATOM	3402	O	ALA	640	62.307	6.608	17.136	1.00	29.82
ATOM	3403	N	ASP	641	64.174	7.456	16.180	1.00	28.74
ATOM	3404	CA	ASP	641	63.863	8.874	16.415	1.00	32.13
ATOM	3405	CB	ASP	641	62.662	9.310	15.574	1.00	35.25
ATOM	3406	CG	ASP	641	63.024	9.555	14.121	1.00	38.54
ATOM	3407	OD1	ASP	641	64.149	9.170	13.716	1.00	39.85
ATOM	3408	OD2	ASP	641	62.192	10.144	13.394	1.00	41.38
ATOM	3409	C	ASP	641	63.661	9.311	17.862	1.00	30.61
ATOM	3410	O	ASP	641	63.012	10.323	18.140	1.00	29.45
ATOM	3411	N	PHE	642	64.265	8.567	18.776	1.00	30.96
ATOM	3412	CA	PHE	642	64.155	8.860	20.195	1.00	31.21
ATOM	3413	CB	PHE	642	64.447	7.597	21.013	1.00	27.06
ATOM	3414	CG	PHE	642	65.806	7.008	20.749	1.00	24.27
ATOM	3415	CD1	PHE	642	66.930	7.476	21.419	1.00	22.36
ATOM	3416	CD2	PHE	642	65.962	5.978	19.838	1.00	24.87
ATOM	3417	CE1	PHE	642	68.179	6.928	21.190	1.00	23.19
ATOM	3418	CE2	PHE	642	67.205	5.420	19.603	1.00	23.65
ATOM	3419	CZ	PHE	642	68.323	5.898	20.282	1.00	22.95
ATOM	3420	C	PHE	642	65.069	10.007	20.623	1.00	34.88
ATOM	3421	O	PHE	642	64.920	10.549	21.729	1.00	34.84
ATOM	3422	N	GLY	643	66.000	10.377	19.737	1.00	36.20
ATOM	3423	CA	GLY	643	66.934	11.450	20.032	1.00	35.47
ATOM	3424	C	GLY	643	66.728	12.720	19.232	1.00	37.62
ATOM	3425	O	GLY	643	67.581	13.593	19.269	1.00	39.16
ATOM	3426	N	LEU	644	65.609	12.837	18.517	1.00	39.68

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ATOM	3427	CA	LEU	644	65.328	14.029	17.712	1.00	43.09
ATOM	3428	CB	LEU	644	64.074	13.843	16.860	1.00	40.78
ATOM	3429	CG	LEU	644	64.076	12.876	15.681	1.00	36.94
ATOM	3430	CD1	LEU	644	62.790	13.076	14.901	1.00	37.34
ATOM	3431	CD2	LEU	644	65.240	13.157	14.783	1.00	37.72
ATOM	3432	C	LEU	644	65.154	15.261	18.591	1.00	47.32
ATOM	3433	O	LEU	644	64.639	15.170	19.702	1.00	50.33
ATOM	3434	N	ALA	645	65.598	16.406	18.088	1.00	51.23
ATOM	3435	CA	ALA	645	65.507	17.662	18.820	1.00	52.97
ATOM	3436	CB	ALA	645	66.367	18.703	18.151	1.00	54.12
ATOM	3437	C	ALA	645	64.060	18.137	18.910	1.00	53.00
ATOM	3438	O	ALA	645	63.591	18.528	19.977	1.00	53.59
ATOM	3439	N	ASP	652	52.356	21.675	14.855	1.00	79.51
ATOM	3440	CA	ASP	652	51.194	21.821	13.993	1.00	78.74
ATOM	3441	CB	ASP	652	51.625	22.021	12.531	1.00	78.30
ATOM	3442	CG	ASP	652	50.459	22.358	11.608	1.00	77.64
ATOM	3443	OD1	ASP	652	49.473	22.968	12.079	1.00	77.67
ATOM	3444	OD2	ASP	652	50.526	22.029	10.410	1.00	78.25
ATOM	3445	C	ASP	652	50.339	20.569	14.125	1.00	78.92
ATOM	3446	O	ASP	652	50.645	19.529	13.539	1.00	79.36
ATOM	3447	N	TYR	653	49.262	20.682	14.892	1.00	79.17
ATOM	3448	CA	TYR	653	48.357	19.560	15.111	1.00	80.23
ATOM	3449	CB	TYR	653	47.283	19.932	16.136	1.00	81.36
ATOM	3450	CG	TYR	653	47.790	20.060	17.557	1.00	84.51
ATOM	3451	CD1	TYR	653	46.998	20.649	18.544	1.00	86.09
ATOM	3452	CE1	TYR	653	47.443	20.751	19.865	1.00	88.05
ATOM	3453	CD2	TYR	653	49.049	19.576	17.925	1.00	86.22
ATOM	3454	CE2	TYR	653	49.504	19.673	19.242	1.00	87.14
ATOM	3455	CZ	TYR	653	48.698	20.260	20.207	1.00	88.37
ATOM	3456	OH	TYR	653	49.146	20.351	21.510	1.00	88.82
ATOM	3457	C	TYR	653	47.687	19.098	13.827	1.00	80.07
ATOM	3458	O	TYR	653	47.170	17.983	13.752	1.00	81.23
ATOM	3459	N	TYR	654	47.716	19.953	12.813	1.00	79.01
ATOM	3460	CA	TYR	654	47.082	19.640	11.544	1.00	78.81
ATOM	3461	CB	TYR	654	46.378	20.884	11.008	1.00	78.48
ATOM	3462	CG	TYR	654	45.358	21.422	11.982	1.00	78.53
ATOM	3463	CD1	TYR	654	45.752	21.948	13.213	1.00	77.46
ATOM	3464	CE1	TYR	654	44.822	22.382	14.146	1.00	78.94
ATOM	3465	CD2	TYR	654	43.997	21.350	11.704	1.00	80.18
ATOM	3466	CE2	TYR	654	43.054	21.785	12.632	1.00	82.55
ATOM	3467	CZ	TYR	654	43.473	22.295	13.851	1.00	80.98
ATOM	3468	OH	TYR	654	42.548	22.703	14.785	1.00	82.29
ATOM	3469	C	TYR	654	48.010	19.042	10.499	1.00	79.04
ATOM	3470	O	TYR	654	47.575	18.720	9.393	1.00	80.09
ATOM	3471	N	LYS	655	49.277	18.859	10.848	1.00	78.74
ATOM	3472	CA	LYS	655	50.217	18.282	9.906	1.00	80.69
ATOM	3473	CB	LYS	655	51.651	18.687	10.247	1.00	83.97
ATOM	3474	CG	LYS	655	52.674	18.124	9.281	1.00	89.76
ATOM	3475	CD	LYS	655	54.084	18.565	9.611	1.00	93.90
ATOM	3476	CE	LYS	655	55.075	17.844	8.708	1.00	97.62
ATOM	3477	NZ	LYS	655	56.489	18.177	9.038	1.00	101.35
ATOM	3478	C	LYS	655	50.070	16.763	9.922	1.00	80.98

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ATOM	3479	O	LYS	655	50.187	16.130	10.975	1.00	80.95
ATOM	3480	N	LYS	656	49.766	16.194	8.759	1.00	81.29
ATOM	3481	CA	LYS	656	49.599	14.749	8.630	1.00	81.06
ATOM	3482	CB	LYS	656	48.723	14.426	7.423	1.00	81.40
ATOM	3483	CG	LYS	656	47.258	14.779	7.596	1.00	81.60
ATOM	3484	CD	LYS	656	46.518	14.565	6.295	1.00	84.93
ATOM	3485	CE	LYS	656	45.019	14.620	6.493	1.00	87.78
ATOM	3486	NZ	LYS	656	44.291	14.565	5.183	1.00	91.78
ATOM	3487	C	LYS	656	50.940	14.026	8.513	1.00	80.44
ATOM	3488	O	LYS	656	51.923	14.596	8.032	1.00	80.35
ATOM	3489	N	GLY	660	49.197	9.779	5.831	1.00	57.41
ATOM	3490	CA	GLY	660	48.231	10.860	5.961	1.00	55.59
ATOM	3491	C	GLY	660	47.492	10.866	7.285	1.00	53.27
ATOM	3492	O	GLY	660	46.403	11.432	7.388	1.00	53.03
ATOM	3493	N	ARG	661	48.080	10.222	8.288	1.00	51.92
ATOM	3494	CA	ARG	661	47.477	10.155	9.617	1.00	48.40
ATOM	3495	CB	ARG	661	47.900	8.861	10.338	1.00	50.20
ATOM	3496	CG	ARG	661	47.612	7.566	9.563	1.00	49.76
ATOM	3497	CD	ARG	661	47.801	6.331	10.456	1.00	52.48
ATOM	3498	NE	ARG	661	47.691	5.061	9.734	1.00	52.60
ATOM	3499	CZ	ARG	661	47.955	3.866	10.264	1.00	50.93
ATOM	3500	NH1	ARG	661	48.343	3.760	11.529	1.00	48.54
ATOM	3501	NH2	ARG	661	47.836	2.772	9.523	1.00	52.75
ATOM	3502	C	ARG	661	47.894	11.379	10.439	1.00	43.81
ATOM	3503	O	ARG	661	48.833	12.096	10.063	1.00	43.23
ATOM	3504	N	LEU	662	47.194	11.618	11.537	1.00	40.56
ATOM	3505	CA	LEU	662	47.496	12.735	12.428	1.00	37.52
ATOM	3506	CB	LEU	662	46.220	13.496	12.789	1.00	33.26
ATOM	3507	CG	LEU	662	45.485	14.281	11.696	1.00	31.29
ATOM	3508	CD1	LEU	662	44.084	14.621	12.158	1.00	24.03
ATOM	3509	CD2	LEU	662	46.261	15.535	11.358	1.00	28.65
ATOM	3510	C	LEU	662	48.154	12.237	13.712	1.00	36.78
ATOM	3511	O	LEU	662	47.515	11.570	14.536	1.00	37.27
ATOM	3512	N	PRO	663	49.448	12.549	13.895	1.00	36.46
ATOM	3513	CD	PRO	663	50.320	13.216	12.914	1.00	38.35
ATOM	3514	CA	PRO	663	50.224	12.148	15.070	1.00	35.98
ATOM	3515	CB	PRO	663	51.537	12.887	14.872	1.00	34.95
ATOM	3516	CG	PRO	663	51.702	12.836	13.403	1.00	39.18
ATOM	3517	C	PRO	663	49.569	12.499	16.398	1.00	35.53
ATOM	3518	O	PRO	663	49.779	11.814	17.399	1.00	38.34
ATOM	3519	N	VAL	664	48.759	13.558	16.414	1.00	32.71
ATOM	3520	CA	VAL	664	48.080	13.964	17.632	1.00	30.18
ATOM	3521	CB	VAL	664	47.195	15.242	17.427	1.00	31.31
ATOM	3522	CG1	VAL	664	48.060	16.409	17.038	1.00	28.93
ATOM	3523	CG2	VAL	664	46.143	15.038	16.345	1.00	34.42
ATOM	3524	C	VAL	664	47.268	12.787	18.172	1.00	29.48
ATOM	3525	O	VAL	664	47.080	12.654	19.388	1.00	30.41
ATOM	3526	N	LYS	665	46.873	11.883	17.282	1.00	29.29
ATOM	3527	CA	LYS	665	46.105	10.704	17.668	1.00	28.55
ATOM	3528	CB	LYS	665	45.517	10.037	16.423	1.00	26.97
ATOM	3529	CG	LYS	665	44.415	10.873	15.786	1.00	27.88
ATOM	3530	CD	LYS	665	43.979	10.366	14.418	1.00	29.41

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ATOM	3531	CE	LYS	665	42.785	11.162	13.899	1.00	26.35
ATOM	3532	NZ	LYS	665	42.363	10.809	12.508	1.00	26.16
ATOM	3533	C	LYS	665	46.890	9.730	18.556	1.00	28.81
ATOM	3534	O	LYS	665	46.315	8.802	19.113	1.00	29.38
ATOM	3535	N	TRP	666	48.181	9.976	18.736	1.00	28.98
ATOM	3536	CA	TRP	666	49.005	9.128	19.599	1.00	31.67
ATOM	3537	CB	TRP	666	50.323	8.755	18.913	1.00	29.46
ATOM	3538	CG	TRP	666	50.205	7.582	17.977	1.00	28.92
ATOM	3539	CD2	TRP	666	49.676	7.603	16.642	1.00	27.62
ATOM	3540	CE2	TRP	666	49.740	6.276	16.162	1.00	27.15
ATOM	3541	CE3	TRP	666	49.151	8.607	15.818	1.00	25.27
ATOM	3542	CD1	TRP	666	50.565	6.289	18.238	1.00	24.30
ATOM	3543	NE1	TRP	666	50.287	5.506	17.147	1.00	27.82
ATOM	3544	CZ2	TRP	666	49.295	5.930	14.872	1.00	26.95
ATOM	3545	CZ3	TRP	666	48.707	8.256	14.536	1.00	25.95
ATOM	3546	CH2	TRP	666	48.778	6.929	14.081	1.00	28.35
ATOM	3547	C	TRP	666	49.316	9.836	20.907	1.00	33.46
ATOM	3548	O	TRP	666	49.790	9.219	21.867	1.00	34.77
ATOM	3549	N	MET	667	49.021	11.128	20.947	1.00	35.61
ATOM	3550	CA	MET	667	49.306	11.948	22.110	1.00	37.94
ATOM	3551	CB	MET	667	49.308	13.419	21.723	1.00	40.22
ATOM	3552	CG	MET	667	50.606	13.939	21.150	1.00	40.77
ATOM	3553	SD	MET	667	50.479	15.723	20.906	1.00	44.04
ATOM	3554	CE	MET	667	50.932	15.858	19.204	1.00	39.07
ATOM	3555	C	MET	667	48.432	11.775	23.346	1.00	39.61
ATOM	3556	O	MET	667	47.211	11.672	23.255	1.00	42.46
ATOM	3557	N	ALA	668	49.072	11.820	24.505	1.00	38.46
ATOM	3558	CA	ALA	668	48.383	11.704	25.773	1.00	37.78
ATOM	3559	CB	ALA	668	49.388	11.473	26.894	1.00	38.21
ATOM	3560	C	ALA	668	47.666	13.033	25.966	1.00	37.46
ATOM	3561	O	ALA	668	48.156	14.072	25.521	1.00	35.74
ATOM	3562	N	PRO	669	46.521	13.027	26.665	1.00	37.55
ATOM	3563	CD	PRO	669	45.868	11.840	27.243	1.00	38.19
ATOM	3564	CA	PRO	669	45.723	14.229	26.923	1.00	39.30
ATOM	3565	CB	PRO	669	44.638	13.708	27.864	1.00	39.82
ATOM	3566	CG	PRO	669	44.444	12.301	27.379	1.00	39.13
ATOM	3567	C	PRO	669	46.517	15.391	27.535	1.00	40.55
ATOM	3568	O	PRO	669	46.442	16.523	27.056	1.00	39.87
ATOM	3569	N	GLU	670	47.303	15.113	28.569	1.00	41.15
ATOM	3570	CA	GLU	670	48.096	16.169	29.200	1.00	42.80
ATOM	3571	CB	GLU	670	48.776	15.657	30.464	1.00	42.97
ATOM	3572	CG	GLU	670	49.928	14.705	30.205	1.00	42.82
ATOM	3573	CD	GLU	670	49.506	13.252	30.150	1.00	44.16
ATOM	3574	OE1	GLU	670	50.395	12.384	30.257	1.00	40.43
ATOM	3575	OE2	GLU	670	48.297	12.974	30.013	1.00	46.36
ATOM	3576	C	GLU	670	49.145	16.795	28.276	1.00	43.00
ATOM	3577	O	GLU	670	49.435	17.979	28.380	1.00	40.37
ATOM	3578	N	ALA	671	49.697	15.999	27.367	1.00	44.03
ATOM	3579	CA	ALA	671	50.708	16.495	26.440	1.00	44.90
ATOM	3580	CB	ALA	671	51.460	15.333	25.814	1.00	42.47
ATOM	3581	C	ALA	671	50.063	17.364	25.361	1.00	47.79
ATOM	3582	O	ALA	671	50.602	18.398	24.977	1.00	47.27

ATOM	3583	N	LEU	672	48.877	16.952	24.922	1.00	51.20
ATOM	3584	CA	LEU	672	48.131	17.650	23.881	1.00	52.90
ATOM	3585	CB	LEU	672	47.092	16.685	23.288	1.00	54.84
ATOM	3586	CG	LEU	672	46.307	17.010	22.015	1.00	57.19
ATOM	3587	CD1	LEU	672	47.230	17.328	20.869	1.00	57.53
ATOM	3588	CD2	LEU	672	45.443	15.813	21.659	1.00	56.95
ATOM	3589	C	LEU	672	47.456	18.913	24.445	1.00	53.45
ATOM	3590	O	LEU	672	47.502	19.988	23.841	1.00	52.71
ATOM	3591	N	PHE	673	46.866	18.777	25.627	1.00	53.82
ATOM	3592	CA	PHE	673	46.179	19.878	26.281	1.00	55.95
ATOM	3593	CB	PHE	673	44.974	19.340	27.060	1.00	53.37
ATOM	3594	CG	PHE	673	43.967	18.612	26.200	1.00	52.79
ATOM	3595	CD1	PHE	673	43.477	17.368	26.580	1.00	54.64
ATOM	3596	CD2	PHE	673	43.491	19.173	25.022	1.00	53.89
ATOM	3597	CE1	PHE	673	42.530	16.702	25.808	1.00	55.44
ATOM	3598	CE2	PHE	673	42.540	18.507	24.239	1.00	54.80
ATOM	3599	CZ	PHE	673	42.062	17.269	24.637	1.00	54.86
ATOM	3600	C	PHE	673	47.071	20.733	27.200	1.00	58.97
ATOM	3601	O	PHE	673	47.084	21.959	27.095	1.00	60.79
ATOM	3602	N	ASP	674	47.832	20.086	28.077	1.00	60.63
ATOM	3603	CA	ASP	674	48.698	20.798	29.026	1.00	61.52
ATOM	3604	CB	ASP	674	48.638	20.137	30.410	1.00	61.39
ATOM	3605	CG	ASP	674	47.247	20.143	31.010	1.00	62.87
ATOM	3606	OD1	ASP	674	46.706	19.039	31.246	1.00	62.99
ATOM	3607	OD2	ASP	674	46.698	21.239	31.253	1.00	63.55
ATOM	3608	C	ASP	674	50.176	20.898	28.618	1.00	61.58
ATOM	3609	O	ASP	674	51.014	21.284	29.446	1.00	60.41
ATOM	3610	N	ARG	675	50.499	20.519	27.380	1.00	61.38
ATOM	3611	CA	ARG	675	51.885	20.526	26.883	1.00	59.23
ATOM	3612	CB	ARG	675	52.336	21.944	26.515	1.00	59.05
ATOM	3613	CG	ARG	675	51.548	22.564	25.367	1.00	64.48
ATOM	3614	CD	ARG	675	52.036	23.967	25.014	1.00	68.61
ATOM	3615	NE	ARG	675	53.348	23.969	24.359	1.00	69.16
ATOM	3616	CZ	ARG	675	54.076	25.061	24.145	1.00	68.19
ATOM	3617	NH1	ARG	675	53.622	26.250	24.531	1.00	66.97
ATOM	3618	NH2	ARG	675	55.265	24.965	23.564	1.00	67.00
ATOM	3619	C	ARG	675	52.849	19.885	27.892	1.00	57.27
ATOM	3620	O	ARG	675	54.002	20.300	28.033	1.00	57.05
ATOM	3621	N	ILE	676	52.356	18.867	28.591	1.00	55.44
ATOM	3622	CA	ILE	676	53.136	18.140	29.589	1.00	53.31
ATOM	3623	CB	ILE	676	52.314	17.899	30.874	1.00	50.96
ATOM	3624	CG2	ILE	676	52.934	16.787	31.718	1.00	47.57
ATOM	3625	CG1	ILE	676	52.213	19.196	31.669	1.00	50.88
ATOM	3626	CD1	ILE	676	51.443	19.073	32.964	1.00	53.09
ATOM	3627	C	ILE	676	53.608	16.801	29.029	1.00	54.75
ATOM	3628	O	ILE	676	52.810	15.891	28.824	1.00	57.06
ATOM	3629	N	TYR	677	54.902	16.681	28.777	1.00	53.61
ATOM	3630	CA	TYR	677	55.459	15.447	28.243	1.00	52.80
ATOM	3631	CB	TYR	677	56.332	15.747	27.023	1.00	53.40
ATOM	3632	CG	TYR	677	55.554	16.184	25.794	1.00	57.32
ATOM	3633	CD1	TYR	677	55.256	17.535	25.575	1.00	55.94
ATOM	3634	CE1	TYR	677	54.574	17.946	24.436	1.00	54.18

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ATOM	3635	CD2	TYR	677	55.140	15.251	24.829	1.00	56.63
ATOM	3636	CE2	TYR	677	54.459	15.654	23.680	1.00	54.84
ATOM	3637	CZ	TYR	677	54.183	17.004	23.490	1.00	56.38
ATOM	3638	OH	TYR	677	53.555	17.426	22.340	1.00	57.46
ATOM	3639	C	TYR	677	56.268	14.713	29.304	1.00	51.49
ATOM	3640	O	TYR	677	57.186	15.283	29.904	1.00	52.65
ATOM	3641	N	THR	678	55.881	13.471	29.579	1.00	48.54
ATOM	3642	CA	THR	678	56.571	12.648	30.568	1.00	46.14
ATOM	3643	CB	THR	678	55.776	12.597	31.910	1.00	47.34
ATOM	3644	OG1	THR	678	54.615	11.764	31.764	1.00	50.96
ATOM	3645	CG2	THR	678	55.346	13.996	32.345	1.00	47.47
ATOM	3646	C	THR	678	56.742	11.218	30.041	1.00	43.21
ATOM	3647	O	THR	678	56.371	10.917	28.912	1.00	41.64
ATOM	3648	N	HIS	679	57.334	10.351	30.854	1.00	42.21
ATOM	3649	CA	HIS	679	57.507	8.969	30.456	1.00	39.96
ATOM	3650	CB	HIS	679	58.410	8.216	31.428	1.00	39.23
ATOM	3651	CG	HIS	679	59.833	8.677	31.418	1.00	43.24
ATOM	3652	CD2	HIS	679	60.501	9.505	32.253	1.00	43.12
ATOM	3653	ND1	HIS	679	60.759	8.236	30.498	1.00	42.63
ATOM	3654	CE1	HIS	679	61.938	8.762	30.774	1.00	42.66
ATOM	3655	NE2	HIS	679	61.807	9.539	31.832	1.00	43.80
ATOM	3656	C	HIS	679	56.145	8.301	30.429	1.00	40.78
ATOM	3657	O	HIS	679	55.930	7.358	29.678	1.00	42.66
ATOM	3658	N	GLN	680	55.227	8.803	31.254	1.00	40.26
ATOM	3659	CA	GLN	680	53.881	8.261	31.324	1.00	39.10
ATOM	3660	CB	GLN	680	53.187	8.664	32.625	1.00	39.23
ATOM	3661	CG	GLN	680	53.762	7.980	33.874	1.00	41.07
ATOM	3662	CD	GLN	680	53.813	6.450	33.770	1.00	39.96
ATOM	3663	OE1	GLN	680	52.818	5.762	33.993	1.00	39.53
ATOM	3664	NE2	GLN	680	54.990	5.919	33.464	1.00	32.85
ATOM	3665	C	GLN	680	53.070	8.676	30.103	1.00	39.20
ATOM	3666	O	GLN	680	52.194	7.933	29.656	1.00	39.29
ATOM	3667	N	SER	681	53.368	9.843	29.531	1.00	38.01
ATOM	3668	CA	SER	681	52.656	10.264	28.325	1.00	39.27
ATOM	3669	CB	SER	681	52.979	11.712	27.968	1.00	40.93
ATOM	3670	OG	SER	681	54.366	11.936	27.943	1.00	39.70
ATOM	3671	C	SER	681	53.090	9.309	27.208	1.00	39.93
ATOM	3672	O	SER	681	52.285	8.953	26.335	1.00	40.46
ATOM	3673	N	ASP	682	54.356	8.881	27.269	1.00	37.28
ATOM	3674	CA	ASP	682	54.920	7.921	26.315	1.00	35.38
ATOM	3675	CB	ASP	682	56.411	7.673	26.586	1.00	33.58
ATOM	3676	CG	ASP	682	57.332	8.520	25.717	1.00	33.16
ATOM	3677	OD1	ASP	682	58.545	8.283	25.828	1.00	31.76
ATOM	3678	OD2	ASP	682	56.886	9.391	24.936	1.00	30.06
ATOM	3679	C	ASP	682	54.178	6.599	26.463	1.00	34.70
ATOM	3680	O	ASP	682	54.012	5.868	25.488	1.00	35.67
ATOM	3681	N	VAL	683	53.758	6.296	27.691	1.00	34.44
ATOM	3682	CA	VAL	683	53.011	5.072	27.987	1.00	35.14
ATOM	3683	CB	VAL	683	52.895	4.852	29.544	1.00	35.48
ATOM	3684	CG1	VAL	683	51.752	3.900	29.890	1.00	34.95
ATOM	3685	CG2	VAL	683	54.202	4.282	30.080	1.00	28.77
ATOM	3686	C	VAL	683	51.638	5.091	27.279	1.00	32.81

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ATOM	3687	O	VAL	683	51.173	4.050	26.801	1.00	31.24
ATOM	3688	N	TRP	684	51.018	6.271	27.187	1.00	30.88
ATOM	3689	CA	TRP	684	49.731	6.426	26.502	1.00	31.79
ATOM	3690	CB	TRP	684	49.189	7.849	26.679	1.00	34.88
ATOM	3691	CG	TRP	684	47.972	8.173	25.833	1.00	37.61
ATOM	3692	CD2	TRP	684	46.635	8.396	26.305	1.00	39.13
ATOM	3693	CE2	TRP	684	45.851	8.741	25.184	1.00	38.42
ATOM	3694	CE3	TRP	684	46.024	8.349	27.567	1.00	39.05
ATOM	3695	CD1	TRP	684	47.938	8.374	24.476	1.00	36.48
ATOM	3696	NE1	TRP	684	46.669	8.720	24.085	1.00	38.70
ATOM	3697	CZ2	TRP	684	44.483	9.036	25.290	1.00	37.82
ATOM	3698	CZ3	TRP	684	44.668	8.644	27.664	1.00	38.19
ATOM	3699	CH2	TRP	684	43.918	8.980	26.536	1.00	37.68
ATOM	3700	C	TRP	684	49.947	6.131	25.020	1.00	31.09
ATOM	3701	O	TRP	684	49.214	5.332	24.430	1.00	32.25
ATOM	3702	N	SER	685	50.977	6.750	24.444	1.00	28.90
ATOM	3703	CA	SER	685	51.345	6.536	23.052	1.00	27.10
ATOM	3704	CB	SER	685	52.620	7.312	22.748	1.00	23.88
ATOM	3705	OG	SER	685	52.459	8.710	22.974	1.00	25.82
ATOM	3706	C	SER	685	51.567	5.028	22.786	1.00	27.85
ATOM	3707	O	SER	685	51.172	4.493	21.746	1.00	28.89
ATOM	3708	N	PHE	686	52.178	4.334	23.741	1.00	28.84
ATOM	3709	CA	PHE	686	52.410	2.893	23.622	1.00	27.86
ATOM	3710	CB	PHE	686	53.255	2.403	24.800	1.00	28.14
ATOM	3711	CG	PHE	686	53.498	0.914	24.803	1.00	28.41
ATOM	3712	CD1	PHE	686	54.256	0.313	23.802	1.00	27.54
ATOM	3713	CD2	PHE	686	52.949	0.109	25.796	1.00	29.15
ATOM	3714	CE1	PHE	686	54.465	-1.057	23.792	1.00	24.25
ATOM	3715	CE2	PHE	686	53.151	-1.268	25.790	1.00	27.86
ATOM	3716	CZ	PHE	686	53.912	-1.850	24.782	1.00	26.09
ATOM	3717	C	PHE	686	51.072	2.122	23.566	1.00	30.99
ATOM	3718	O	PHE	686	50.960	1.109	22.873	1.00	29.21
ATOM	3719	N	GLY	687	50.051	2.603	24.286	1.00	30.57
ATOM	3720	CA	GLY	687	48.758	1.939	24.273	1.00	31.78
ATOM	3721	C	GLY	687	48.202	1.923	22.862	1.00	32.51
ATOM	3722	O	GLY	687	47.687	0.908	22.373	1.00	31.25
ATOM	3723	N	VAL	688	48.292	3.073	22.204	1.00	32.58
ATOM	3724	CA	VAL	688	47.825	3.202	20.827	1.00	30.66
ATOM	3725	CB	VAL	688	47.804	4.684	20.362	1.00	28.55
ATOM	3726	CG1	VAL	688	47.231	4.795	18.950	1.00	27.25
ATOM	3727	CG2	VAL	688	46.944	5.522	21.320	1.00	27.12
ATOM	3728	C	VAL	688	48.684	2.326	19.910	1.00	29.96
ATOM	3729	O	VAL	688	48.160	1.731	18.974	1.00	30.83
ATOM	3730	N	LEU	689	49.973	2.202	20.219	1.00	30.02
ATOM	3731	CA	LEU	689	50.893	1.371	19.430	1.00	30.48
ATOM	3732	CB	LEU	689	52.359	1.571	19.877	1.00	28.13
ATOM	3733	CG	LEU	689	53.466	0.966	18.995	1.00	26.34
ATOM	3734	CD1	LEU	689	54.790	1.697	19.174	1.00	25.54
ATOM	3735	CD2	LEU	689	53.628	-0.505	19.264	1.00	24.99
ATOM	3736	C	LEU	689	50.479	-0.096	19.567	1.00	30.54
ATOM	3737	O	LEU	689	50.540	-0.849	18.602	1.00	27.86
ATOM	3738	N	LEU	690	50.013	-0.468	20.759	1.00	33.73

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ATOM	3739	CA	LEU	690	49.553	-1.830	21.029	1.00	32.47
ATOM	3740	CB	LEU	690	49.141	-1.982	22.496	1.00	31.82
ATOM	3741	CG	LEU	690	50.136	-2.220	23.634	1.00	29.71
ATOM	3742	CD1	LEU	690	49.396	-2.129	24.956	1.00	31.53
ATOM	3743	CD2	LEU	690	50.771	-3.605	23.483	1.00	31.69
ATOM	3744	C	LEU	690	48.335	-2.101	20.136	1.00	33.01
ATOM	3745	O	LEU	690	48.223	-3.168	19.521	1.00	32.68
ATOM	3746	N	TRP	691	47.423	-1.131	20.089	1.00	32.37
ATOM	3747	CA	TRP	691	46.230	-1.215	19.256	1.00	32.11
ATOM	3748	CB	TRP	691	45.424	0.083	19.373	1.00	33.19
ATOM	3749	CG	TRP	691	44.086	0.055	18.678	1.00	33.95
ATOM	3750	CD2	TRP	691	43.812	0.469	17.337	1.00	30.48
ATOM	3751	CE2	TRP	691	42.434	0.294	17.118	1.00	32.75
ATOM	3752	CE3	TRP	691	44.599	0.989	16.301	1.00	29.47
ATOM	3753	CD1	TRP	691	42.889	-0.352	19.199	1.00	34.34
ATOM	3754	NE1	TRP	691	41.894	-0.211	18.272	1.00	36.53
ATOM	3755	CZ2	TRP	691	41.831	0.601	15.900	1.00	30.85
ATOM	3756	CZ3	TRP	691	44.003	1.289	15.100	1.00	30.51
ATOM	3757	CH2	TRP	691	42.630	1.104	14.907	1.00	30.29
ATOM	3758	C	TRP	691	46.661	-1.421	17.805	1.00	31.49
ATOM	3759	O	TRP	691	46.062	-2.221	17.092	1.00	31.20
ATOM	3760	N	GLU	692	47.669	-0.656	17.374	1.00	32.90
ATOM	3761	CA	GLU	692	48.207	-0.734	16.019	1.00	29.78
ATOM	3762	CB	GLU	692	49.383	0.233	15.809	1.00	25.56
ATOM	3763	CG	GLU	692	49.009	1.696	15.713	1.00	25.85
ATOM	3764	CD	GLU	692	50.195	2.570	15.363	1.00	27.76
ATOM	3765	OE1	GLU	692	51.001	2.850	16.265	1.00	29.52
ATOM	3766	OE2	GLU	692	50.333	2.981	14.191	1.00	26.84
ATOM	3767	C	GLU	692	48.682	-2.136	15.696	1.00	31.08
ATOM	3768	O	GLU	692	48.545	-2.593	14.553	1.00	32.57
ATOM	3769	N	ILE	693	49.262	-2.804	16.689	1.00	31.81
ATOM	3770	CA	ILE	693	49.774	-4.163	16.506	1.00	31.87
ATOM	3771	CB	ILE	693	50.666	-4.614	17.699	1.00	33.50
ATOM	3772	CG2	ILE	693	51.140	-6.075	17.513	1.00	33.06
ATOM	3773	CG1	ILE	693	51.879	-3.703	17.827	1.00	34.04
ATOM	3774	CD1	ILE	693	52.744	-4.008	19.025	1.00	31.52
ATOM	3775	C	ILE	693	48.643	-5.177	16.335	1.00	31.43
ATOM	3776	O	ILE	693	48.633	-5.982	15.403	1.00	29.55
ATOM	3777	N	PHE	694	47.654	-5.087	17.207	1.00	33.58
ATOM	3778	CA	PHE	694	46.550	-6.027	17.178	1.00	36.72
ATOM	3779	CB	PHE	694	45.980	-6.179	18.589	1.00	36.27
ATOM	3780	CG	PHE	694	46.988	-6.724	19.547	1.00	34.29
ATOM	3781	CD1	PHE	694	47.500	-5.949	20.581	1.00	34.95
ATOM	3782	CD2	PHE	694	47.560	-7.972	19.297	1.00	31.60
ATOM	3783	CE1	PHE	694	48.576	-6.413	21.344	1.00	35.73
ATOM	3784	CE2	PHE	694	48.633	-8.443	20.049	1.00	31.12
ATOM	3785	CZ	PHE	694	49.149	-7.661	21.066	1.00	33.97
ATOM	3786	C	PHE	694	45.516	-5.870	16.065	1.00	37.70
ATOM	3787	O	PHE	694	44.684	-6.756	15.839	1.00	37.99
ATOM	3788	N	THR	695	45.604	-4.745	15.355	1.00	36.11
ATOM	3789	CA	THR	695	44.747	-4.485	14.205	1.00	31.23
ATOM	3790	CB	THR	695	44.107	-3.081	14.236	1.00	30.49

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ATOM	3791	OG1	THR	695	45.133	-2.079	14.134	1.00	30.14
ATOM	3792	CG2	THR	695	43.329	-2.888	15.512	1.00	31.07
ATOM	3793	C	THR	695	45.612	-4.619	12.965	1.00	29.79
ATOM	3794	O	THR	695	45.163	-4.325	11.862	1.00	31.31
ATOM	3795	N	LEU	696	46.859	-5.051	13.164	1.00	29.75
ATOM	3796	CA	LEU	696	47.826	-5.259	12.081	1.00	28.46
ATOM	3797	CB	LEU	696	47.456	-6.495	11.245	1.00	29.96
ATOM	3798	CG	LEU	696	47.281	-7.848	11.946	1.00	30.38
ATOM	3799	CD1	LEU	696	47.142	-8.941	10.909	1.00	30.43
ATOM	3800	CD2	LEU	696	48.468	-8.138	12.800	1.00	32.35
ATOM	3801	C	LEU	696	48.101	-4.076	11.160	1.00	28.76
ATOM	3802	O	LEU	696	48.210	-4.235	9.946	1.00	26.97
ATOM	3803	N	GLY	697	48.314	-2.900	11.745	1.00	32.70
ATOM	3804	CA	GLY	697	48.609	-1.705	10.960	1.00	31.69
ATOM	3805	C	GLY	697	47.432	-0.763	10.817	1.00	32.24
ATOM	3806	O	GLY	697	47.398	0.099	9.941	1.00	31.81
ATOM	3807	N	GLY	698	46.455	-0.922	11.700	1.00	32.63
ATOM	3808	CA	GLY	698	45.277	-0.081	11.643	1.00	31.93
ATOM	3809	C	GLY	698	45.504	1.411	11.820	1.00	28.95
ATOM	3810	O	GLY	698	46.454	1.858	12.449	1.00	26.05
ATOM	3811	N	SER	699	44.569	2.174	11.282	1.00	30.03
ATOM	3812	CA	SER	699	44.608	3.618	11.352	1.00	30.52
ATOM	3813	CB	SER	699	44.095	4.219	10.046	1.00	31.24
ATOM	3814	OG	SER	699	44.047	5.639	10.095	1.00	33.61
ATOM	3815	C	SER	699	43.695	4.024	12.492	1.00	30.45
ATOM	3816	O	SER	699	42.490	3.755	12.450	1.00	29.11
ATOM	3817	N	PRO	700	44.259	4.591	13.573	1.00	32.27
ATOM	3818	CD	PRO	700	45.693	4.761	13.881	1.00	29.61
ATOM	3819	CA	PRO	700	43.408	5.007	14.695	1.00	31.34
ATOM	3820	CB	PRO	700	44.428	5.358	15.777	1.00	31.30
ATOM	3821	CG	PRO	700	45.662	5.745	14.989	1.00	29.66
ATOM	3822	C	PRO	700	42.574	6.208	14.279	1.00	29.65
ATOM	3823	O	PRO	700	43.032	7.062	13.527	1.00	30.44
ATOM	3824	N	TYR	701	41.306	6.190	14.660	1.00	30.37
ATOM	3825	CA	TYR	701	40.359	7.272	14.367	1.00	30.01
ATOM	3826	CB	TYR	701	40.655	8.474	15.269	1.00	35.19
ATOM	3827	CG	TYR	701	40.452	8.215	16.749	1.00	39.32
ATOM	3828	CD1	TYR	701	41.452	8.518	17.675	1.00	43.08
ATOM	3829	CE1	TYR	701	41.258	8.305	19.041	1.00	46.20
ATOM	3830	CD2	TYR	701	39.256	7.688	17.229	1.00	40.66
ATOM	3831	CE2	TYR	701	39.060	7.469	18.584	1.00	43.51
ATOM	3832	CZ	TYR	701	40.056	7.782	19.485	1.00	45.75
ATOM	3833	OH	TYR	701	39.847	7.592	20.837	1.00	50.92
ATOM	3834	C	TYR	701	40.273	7.722	12.909	1.00	29.04
ATOM	3835	O	TYR	701	40.393	8.904	12.611	1.00	28.53
ATOM	3836	N	PRO	702	40.015	6.777	11.986	1.00	28.69
ATOM	3837	CD	PRO	702	39.761	5.346	12.186	1.00	26.94
ATOM	3838	CA	PRO	702	39.920	7.145	10.569	1.00	27.55
ATOM	3839	CB	PRO	702	39.709	5.800	9.882	1.00	27.91
ATOM	3840	CG	PRO	702	39.054	4.971	10.917	1.00	29.04
ATOM	3841	C	PRO	702	38.790	8.117	10.264	1.00	29.20
ATOM	3842	O	PRO	702	37.631	7.880	10.617	1.00	32.39

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ATOM	3843	N	GLY	703	39.148	9.213	9.591	1.00	28.34
ATOM	3844	CA	GLY	703	38.191	10.236	9.226	1.00	25.97
ATOM	3845	C	GLY	703	37.960	11.289	10.297	1.00	28.00
ATOM	3846	O	GLY	703	37.175	12.213	10.079	1.00	26.40
ATOM	3847	N	VAL	704	38.621	11.139	11.448	1.00	29.54
ATOM	3848	CA	VAL	704	38.480	12.061	12.576	1.00	30.61
ATOM	3849	CB	VAL	704	38.606	11.324	13.944	1.00	32.54
ATOM	3850	CG1	VAL	704	38.577	12.324	15.111	1.00	31.95
ATOM	3851	CG2	VAL	704	37.482	10.311	14.103	1.00	34.62
ATOM	3852	C	VAL	704	39.490	13.210	12.557	1.00	31.37
ATOM	3853	O	VAL	704	40.683	13.001	12.757	1.00	31.73
ATOM	3854	N	PRO	705	39.030	14.430	12.281	1.00	32.70
ATOM	3855	CD	PRO	705	37.669	14.770	11.819	1.00	33.75
ATOM	3856	CA	PRO	705	39.910	15.599	12.243	1.00	31.90
ATOM	3857	CB	PRO	705	39.065	16.641	11.518	1.00	32.66
ATOM	3858	CG	PRO	705	37.674	16.273	11.906	1.00	35.32
ATOM	3859	C	PRO	705	40.331	16.053	13.635	1.00	31.85
ATOM	3860	O	PRO	705	39.709	15.686	14.634	1.00	31.50
ATOM	3861	N	VAL	706	41.372	16.879	13.676	1.00	32.32
ATOM	3862	CA	VAL	706	41.945	17.389	14.925	1.00	36.88
ATOM	3863	CB	VAL	706	42.991	18.505	14.664	1.00	39.77
ATOM	3864	CG1	VAL	706	43.657	18.907	15.974	1.00	39.17
ATOM	3865	CG2	VAL	706	44.035	18.057	13.618	1.00	38.70
ATOM	3866	C	VAL	706	40.938	17.923	15.953	1.00	37.80
ATOM	3867	O	VAL	706	40.994	17.581	17.140	1.00	37.45
ATOM	3868	N	GLU	707	39.991	18.724	15.483	1.00	38.19
ATOM	3869	CA	GLU	707	39.009	19.308	16.370	1.00	37.31
ATOM	3870	CB	GLU	707	38.208	20.361	15.619	1.00	37.46
ATOM	3871	C	GLU	707	38.084	18.264	16.994	1.00	39.56
ATOM	3872	O	GLU	707	37.739	18.344	18.177	1.00	41.39
ATOM	3873	N	GLU	708	37.724	17.260	16.206	1.00	39.99
ATOM	3874	CA	GLU	708	36.840	16.212	16.684	1.00	40.08
ATOM	3875	CB	GLU	708	36.334	15.377	15.515	1.00	43.96
ATOM	3876	CG	GLU	708	35.505	16.163	14.496	1.00	46.61
ATOM	3877	CD	GLU	708	34.288	16.851	15.099	1.00	52.77
ATOM	3878	OE1	GLU	708	33.659	16.305	16.040	1.00	52.52
ATOM	3879	OE2	GLU	708	33.954	17.955	14.604	1.00	57.04
ATOM	3880	C	GLU	708	37.551	15.337	17.704	1.00	39.89
ATOM	3881	O	GLU	708	36.944	14.900	18.684	1.00	39.47
ATOM	3882	N	LEU	709	38.838	15.086	17.471	1.00	38.99
ATOM	3883	CA	LEU	709	39.638	14.277	18.393	1.00	37.51
ATOM	3884	CB	LEU	709	41.079	14.120	17.892	1.00	34.15
ATOM	3885	CG	LEU	709	42.061	13.338	18.787	1.00	30.94
ATOM	3886	CD1	LEU	709	41.861	11.834	18.689	1.00	28.48
ATOM	3887	CD2	LEU	709	43.459	13.712	18.395	1.00	29.02
ATOM	3888	C	LEU	709	39.644	14.961	19.751	1.00	38.18
ATOM	3889	O	LEU	709	39.460	14.313	20.787	1.00	38.08
ATOM	3890	N	PHE	710	39.833	16.276	19.749	1.00	39.68
ATOM	3891	CA	PHE	710	39.845	17.021	21.001	1.00	43.27
ATOM	3892	CB	PHE	710	40.024	18.524	20.747	1.00	43.66
ATOM	3893	CG	PHE	710	41.376	18.888	20.225	1.00	46.36
ATOM	3894	CD1	PHE	710	42.459	18.024	20.403	1.00	48.33

ATOM	3895	CD2	PHE	710	41.579	20.084	19.544	1.00	47.76
ATOM	3896	CE1	PHE	710	43.723	18.343	19.915	1.00	51.79
ATOM	3897	CE2	PHE	710	42.839	20.417	19.046	1.00	50.36
ATOM	3898	CZ	PHE	710	43.916	19.544	19.233	1.00	53.02
ATOM	3899	C	PHE	710	38.558	16.746	21.758	1.00	44.74
ATOM	3900	O	PHE	710	38.587	16.422	22.952	1.00	44.99
ATOM	3901	N	LYS	711	37.445	16.777	21.032	1.00	45.27
ATOM	3902	CA	LYS	711	36.146	16.529	21.627	1.00	44.00
ATOM	3903	CB	LYS	711	35.031	16.870	20.634	1.00	46.68
ATOM	3904	CG	LYS	711	33.645	16.758	21.235	1.00	52.36
ATOM	3905	CD	LYS	711	32.556	17.224	20.293	1.00	54.43
ATOM	3906	CE	LYS	711	31.197	16.809	20.826	1.00	55.93
ATOM	3907	NZ	LYS	711	30.101	17.220	19.912	1.00	63.51
ATOM	3908	C	LYS	711	36.052	15.078	22.120	1.00	42.15
ATOM	3909	O	LYS	711	35.635	14.827	23.250	1.00	40.85
ATOM	3910	N	LEU	712	36.467	14.125	21.294	1.00	40.98
ATOM	3911	CA	LEU	712	36.432	12.719	21.691	1.00	42.26
ATOM	3912	CB	LEU	712	37.012	11.814	20.597	1.00	39.67
ATOM	3913	CG	LEU	712	36.159	11.449	19.381	1.00	39.06
ATOM	3914	CD1	LEU	712	36.899	10.440	18.504	1.00	36.97
ATOM	3915	CD2	LEU	712	34.842	10.868	19.857	1.00	36.48
ATOM	3916	C	LEU	712	37.232	12.513	22.974	1.00	43.61
ATOM	3917	O	LEU	712	36.796	11.785	23.875	1.00	44.10
ATOM	3918	N	LEU	713	38.407	13.141	23.038	1.00	43.57
ATOM	3919	CA	LEU	713	39.271	13.034	24.207	1.00	43.67
ATOM	3920	CB	LEU	713	40.619	13.726	23.958	1.00	42.24
ATOM	3921	CG	LEU	713	41.569	13.004	22.989	1.00	38.81
ATOM	3922	CD1	LEU	713	42.856	13.796	22.817	1.00	30.86
ATOM	3923	CD2	LEU	713	41.873	11.591	23.519	1.00	34.27
ATOM	3924	C	LEU	713	38.589	13.594	25.450	1.00	44.78
ATOM	3925	O	LEU	713	38.548	12.919	26.472	1.00	46.04
ATOM	3926	N	LYS	714	38.002	14.785	25.344	1.00	44.72
ATOM	3927	CA	LYS	714	37.304	15.394	26.471	1.00	44.34
ATOM	3928	CB	LYS	714	36.818	16.799	26.114	1.00	43.76
ATOM	3929	CG	LYS	714	37.955	17.761	25.926	1.00	46.37
ATOM	3930	CD	LYS	714	37.497	19.174	25.628	1.00	52.22
ATOM	3931	CE	LYS	714	38.701	20.044	25.235	1.00	57.37
ATOM	3932	NZ	LYS	714	39.792	20.059	26.279	1.00	58.02
ATOM	3933	C	LYS	714	36.142	14.534	26.972	1.00	44.17
ATOM	3934	O	LYS	714	35.861	14.499	28.167	1.00	45.14
ATOM	3935	N	GLU	715	35.498	13.809	26.068	1.00	43.86
ATOM	3936	CA	GLU	715	34.392	12.935	26.430	1.00	42.94
ATOM	3937	CB	GLU	715	33.518	12.652	25.195	1.00	46.57
ATOM	3938	CG	GLU	715	32.930	13.897	24.532	1.00	51.37
ATOM	3939	CD	GLU	715	32.032	13.571	23.338	1.00	54.24
ATOM	3940	OE1	GLU	715	32.215	12.503	22.704	1.00	54.19
ATOM	3941	OE2	GLU	715	31.139	14.392	23.033	1.00	55.01
ATOM	3942	C	GLU	715	34.878	11.607	27.036	1.00	41.36
ATOM	3943	O	GLU	715	34.076	10.730	27.348	1.00	38.24
ATOM	3944	N	GLY	716	36.184	11.452	27.182	1.00	41.41
ATOM	3945	CA	GLY	716	36.727	10.225	27.737	1.00	41.78
ATOM	3946	C	GLY	716	36.602	9.034	26.799	1.00	42.65

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ATOM	3947	O	GLY	716	36.661	7.874	27.225	1.00	41.41
ATOM	3948	N	HIS	717	36.439	9.321	25.513	1.00	44.56
ATOM	3949	CA	HIS	717	36.286	8.291	24.502	1.00	45.91
ATOM	3950	CB	HIS	717	35.935	8.926	23.153	1.00	46.65
ATOM	3951	CG	HIS	717	35.860	7.946	22.024	1.00	50.03
ATOM	3952	CD2	HIS	717	34.842	7.171	21.581	1.00	49.92
ATOM	3953	ND1	HIS	717	36.946	7.634	21.235	1.00	51.38
ATOM	3954	CE1	HIS	717	36.604	6.708	20.360	1.00	50.10
ATOM	3955	NE2	HIS	717	35.335	6.408	20.550	1.00	49.34
ATOM	3956	C	HIS	717	37.535	7.434	24.354	1.00	47.68
ATOM	3957	O	HIS	717	38.649	7.949	24.287	1.00	49.77
ATOM	3958	N	ARG	718	37.328	6.118	24.283	1.00	48.18
ATOM	3959	CA	ARG	718	38.403	5.148	24.116	1.00	46.95
ATOM	3960	CB	ARG	718	38.571	4.307	25.385	1.00	45.75
ATOM	3961	CG	ARG	718	38.945	5.125	26.618	1.00	47.15
ATOM	3962	CD	ARG	718	40.273	5.852	26.420	1.00	46.61
ATOM	3963	NE	ARG	718	40.722	6.579	27.608	1.00	45.57
ATOM	3964	CZ	ARG	718	40.601	7.896	27.779	1.00	45.48
ATOM	3965	NH1	ARG	718	40.033	8.644	26.845	1.00	44.14
ATOM	3966	NH2	ARG	718	41.122	8.480	28.854	1.00	43.32
ATOM	3967	C	ARG	718	38.109	4.250	22.912	1.00	47.56
ATOM	3968	O	ARG	718	36.946	3.991	22.589	1.00	48.37
ATOM	3969	N	MET	719	39.149	3.873	22.181	1.00	47.33
ATOM	3970	CA	MET	719	38.984	3.021	21.013	1.00	47.90
ATOM	3971	CB	MET	719	40.282	2.939	20.198	1.00	47.21
ATOM	3972	CG	MET	719	40.652	4.245	19.509	1.00	45.79
ATOM	3973	SD	MET	719	42.095	4.104	18.440	1.00	42.81
ATOM	3974	CE	MET	719	43.377	3.970	19.604	1.00	43.02
ATOM	3975	C	MET	719	38.519	1.629	21.392	1.00	49.99
ATOM	3976	O	MET	719	38.889	1.102	22.450	1.00	47.98
ATOM	3977	N	ASP	720	37.690	1.050	20.523	1.00	53.40
ATOM	3978	CA	ASP	720	37.135	-0.288	20.722	1.00	53.19
ATOM	3979	CB	ASP	720	36.089	-0.638	19.647	1.00	56.95
ATOM	3980	CG	ASP	720	34.916	0.333	19.605	1.00	61.65
ATOM	3981	OD1	ASP	720	34.908	1.331	20.356	1.00	68.60
ATOM	3982	OD2	ASP	720	33.996	0.095	18.792	1.00	61.19
ATOM	3983	C	ASP	720	38.208	-1.372	20.713	1.00	51.12
ATOM	3984	O	ASP	720	39.263	-1.229	20.081	1.00	50.71
ATOM	3985	N	LYS	721	37.926	-2.453	21.432	1.00	48.85
ATOM	3986	CA	LYS	721	38.833	-3.576	21.509	1.00	47.92
ATOM	3987	CB	LYS	721	38.335	-4.560	22.562	1.00	47.79
ATOM	3988	CG	LYS	721	39.024	-5.901	22.521	1.00	51.08
ATOM	3989	CD	LYS	721	38.493	-6.810	23.597	1.00	53.21
ATOM	3990	CE	LYS	721	38.484	-8.255	23.141	1.00	54.60
ATOM	3991	NZ	LYS	721	38.158	-9.176	24.268	1.00	61.37
ATOM	3992	C	LYS	721	38.861	-4.261	20.155	1.00	49.01
ATOM	3993	O	LYS	721	37.822	-4.688	19.653	1.00	52.79
ATOM	3994	N	PRO	722	40.053	-4.366	19.541	1.00	48.92
ATOM	3995	CD	PRO	722	41.356	-3.839	19.972	1.00	51.11
ATOM	3996	CA	PRO	722	40.167	-5.011	18.233	1.00	46.01
ATOM	3997	CB	PRO	722	41.663	-4.904	17.918	1.00	45.64
ATOM	3998	CG	PRO	722	42.090	-3.690	18.646	1.00	47.86

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ATOM	3999	C	PRO	722	39.745	-6.466	18.303	1.00	43.57
ATOM	4000	O	PRO	722	39.719	-7.069	19.381	1.00	41.72
ATOM	4001	N	SER	723	39.360	-7.001	17.150	1.00	43.14
ATOM	4002	CA	SER	723	38.991	-8.398	17.044	1.00	41.85
ATOM	4003	CB	SER	723	38.260	-8.660	15.734	1.00	37.27
ATOM	4004	OG	SER	723	39.112	-8.421	14.639	1.00	39.44
ATOM	4005	C	SER	723	40.339	-9.110	17.049	1.00	41.68
ATOM	4006	O	SER	723	41.299	-8.605	16.493	1.00	40.84
ATOM	4007	N	ASN	724	40.405	-10.275	17.683	1.00	45.99
ATOM	4008	CA	ASN	724	41.651	-11.034	17.800	1.00	49.22
ATOM	4009	CB	ASN	724	42.342	-11.215	16.453	1.00	52.35
ATOM	4010	CG	ASN	724	41.768	-12.357	15.668	1.00	58.07
ATOM	4011	OD1	ASN	724	41.821	-13.506	16.103	1.00	62.42
ATOM	4012	ND2	ASN	724	41.186	-12.054	14.513	1.00	62.13
ATOM	4013	C	ASN	724	42.558	-10.323	18.787	1.00	49.77
ATOM	4014	O	ASN	724	43.698	-9.982	18.494	1.00	51.48
ATOM	4015	N	CYS	725	41.995	-10.054	19.954	1.00	50.34
ATOM	4016	CA	CYS	725	42.698	-9.398	21.028	1.00	49.83
ATOM	4017	CB	CYS	725	42.623	-7.878	20.868	1.00	47.11
ATOM	4018	SG	CYS	725	43.485	-6.992	22.169	1.00	38.55
ATOM	4019	C	CYS	725	42.001	-9.861	22.299	1.00	50.11
ATOM	4020	O	CYS	725	40.772	-9.852	22.383	1.00	50.63
ATOM	4021	N	THR	726	42.788	-10.350	23.244	1.00	50.37
ATOM	4022	CA	THR	726	42.261	-10.843	24.497	1.00	51.05
ATOM	4023	CB	THR	726	43.341	-11.663	25.234	1.00	53.50
ATOM	4024	OG1	THR	726	44.292	-10.780	25.829	1.00	57.56
ATOM	4025	CG2	THR	726	44.074	-12.554	24.241	1.00	52.55
ATOM	4026	C	THR	726	41.843	-9.665	25.354	1.00	52.18
ATOM	4027	O	THR	726	42.403	-8.574	25.219	1.00	55.14
ATOM	4028	N	ASN	727	40.868	-9.860	26.237	1.00	52.55
ATOM	4029	CA	ASN	727	40.401	-8.781	27.114	1.00	53.17
ATOM	4030	CB	ASN	727	39.246	-9.265	27.992	1.00	60.65
ATOM	4031	CG	ASN	727	39.584	-10.545	28.751	1.00	68.99
ATOM	4032	OD1	ASN	727	40.704	-10.718	29.243	1.00	73.66
ATOM	4033	ND2	ASN	727	38.629	-11.454	28.825	1.00	74.66
ATOM	4034	C	ASN	727	41.537	-8.254	27.976	1.00	50.79
ATOM	4035	O	ASN	727	41.513	-7.107	28.414	1.00	48.17
ATOM	4036	N	GLU	728	42.527	-9.111	28.215	1.00	50.18
ATOM	4037	CA	GLU	728	43.693	-8.764	29.020	1.00	49.68
ATOM	4038	CB	GLU	728	44.544	-10.011	29.289	1.00	50.61
ATOM	4039	CG	GLU	728	45.801	-9.758	30.120	1.00	55.44
ATOM	4040	CD	GLU	728	46.509	-11.045	30.542	1.00	56.45
ATOM	4041	OE1	GLU	728	46.737	-11.930	29.685	1.00	53.73
ATOM	4042	OE2	GLU	728	46.865	-11.161	31.733	1.00	57.38
ATOM	4043	C	GLU	728	44.509	-7.713	28.272	1.00	46.92
ATOM	4044	O	GLU	728	44.760	-6.614	28.785	1.00	46.08
ATOM	4045	N	LEU	729	44.869	-8.039	27.033	1.00	42.69
ATOM	4046	CA	LEU	729	45.641	-7.137	26.192	1.00	40.42
ATOM	4047	CB	LEU	729	45.950	-7.796	24.846	1.00	34.84
ATOM	4048	CG	LEU	729	47.004	-8.900	24.952	1.00	34.35
ATOM	4049	CD1	LEU	729	46.960	-9.780	23.749	1.00	31.03
ATOM	4050	CD2	LEU	729	48.404	-8.320	25.139	1.00	33.63

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ATOM	4051	C	LEU	729	44.909	-5.817	25.985	1.00	40.58
ATOM	4052	O	LEU	729	45.524	-4.760	25.929	1.00	40.10
ATOM	4053	N	TYR	730	43.591	-5.886	25.917	1.00	39.32
ATOM	4054	CA	TYR	730	42.807	-4.694	25.720	1.00	41.49
ATOM	4055	CB	TYR	730	41.384	-5.052	25.302	1.00	39.70
ATOM	4056	CG	TYR	730	40.507	-3.846	25.099	1.00	39.53
ATOM	4057	CD1	TYR	730	40.828	-2.879	24.142	1.00	35.10
ATOM	4058	CE1	TYR	730	40.019	-1.758	23.958	1.00	36.33
ATOM	4059	CD2	TYR	730	39.352	-3.661	25.874	1.00	38.44
ATOM	4060	CE2	TYR	730	38.537	-2.541	25.696	1.00	37.68
ATOM	4061	CZ	TYR	730	38.876	-1.601	24.730	1.00	36.85
ATOM	4062	OH	TYR	730	38.041	-0.541	24.489	1.00	40.58
ATOM	4063	C	TYR	730	42.814	-3.849	26.993	1.00	43.50
ATOM	4064	O	TYR	730	42.880	-2.621	26.931	1.00	44.45
ATOM	4065	N	MET	731	42.753	-4.492	28.151	1.00	46.53
ATOM	4066	CA	MET	731	42.782	-3.744	29.406	1.00	48.67
ATOM	4067	CB	MET	731	42.488	-4.668	30.590	1.00	54.90
ATOM	4068	CG	MET	731	41.072	-5.229	30.577	1.00	63.75
ATOM	4069	SD	MET	731	39.766	-3.998	30.763	1.00	69.82
ATOM	4070	CE	MET	731	39.849	-3.788	32.581	1.00	68.20
ATOM	4071	C	MET	731	44.148	-3.087	29.551	1.00	45.73
ATOM	4072	O	MET	731	44.273	-2.024	30.160	1.00	42.09
ATOM	4073	N	MET	732	45.168	-3.728	28.986	1.00	43.47
ATOM	4074	CA	MET	732	46.519	-3.189	29.024	1.00	43.85
ATOM	4075	CB	MET	732	47.515	-4.154	28.365	1.00	40.67
ATOM	4076	CG	MET	732	48.966	-3.646	28.369	1.00	39.96
ATOM	4077	SD	MET	732	50.252	-4.870	27.887	1.00	35.34
ATOM	4078	CE	MET	732	50.523	-5.667	29.390	1.00	35.15
ATOM	4079	C	MET	732	46.460	-1.860	28.275	1.00	43.91
ATOM	4080	O	MET	732	46.924	-0.835	28.782	1.00	47.29
ATOM	4081	N	MET	733	45.798	-1.860	27.120	1.00	42.51
ATOM	4082	CA	MET	733	45.639	-0.652	26.319	1.00	39.85
ATOM	4083	CB	MET	733	44.888	-0.932	25.013	1.00	38.08
ATOM	4084	CG	MET	733	45.614	-1.805	23.991	1.00	37.14
ATOM	4085	SD	MET	733	44.509	-2.170	22.578	1.00	37.32
ATOM	4086	CE	MET	733	45.198	-3.684	21.929	1.00	28.98
ATOM	4087	C	MET	733	44.838	0.363	27.123	1.00	41.12
ATOM	4088	O	MET	733	45.228	1.532	27.213	1.00	44.38
ATOM	4089	N	ARG	734	43.737	-0.084	27.731	1.00	40.28
ATOM	4090	CA	ARG	734	42.893	0.813	28.516	1.00	40.23
ATOM	4091	CB	ARG	734	41.632	0.095	29.007	1.00	39.95
ATOM	4092	CG	ARG	734	40.723	-0.384	27.894	1.00	36.41
ATOM	4093	CD	ARG	734	40.323	0.741	26.995	1.00	39.31
ATOM	4094	NE	ARG	734	39.510	1.733	27.682	1.00	48.97
ATOM	4095	CZ	ARG	734	38.182	1.681	27.774	1.00	53.99
ATOM	4096	NH1	ARG	734	37.503	0.681	27.222	1.00	56.64
ATOM	4097	NH2	ARG	734	37.526	2.633	28.416	1.00	56.79
ATOM	4098	C	ARG	734	43.694	1.387	29.675	1.00	39.38
ATOM	4099	O	ARG	734	43.538	2.564	30.010	1.00	41.82
ATOM	4100	N	ASP	735	44.583	0.572	30.244	1.00	37.67
ATOM	4101	CA	ASP	735	45.465	1.000	31.339	1.00	39.58
ATOM	4102	CB	ASP	735	46.392	-0.137	31.773	1.00	42.90

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ATOM	4103	CG	ASP	735	45.690	-1.175	32.604	1.00	47.78
ATOM	4104	OD1	ASP	735	46.116	-2.355	32.524	1.00	47.92
ATOM	4105	OD2	ASP	735	44.733	-0.803	33.339	1.00	46.75
ATOM	4106	C	ASP	735	46.339	2.161	30.881	1.00	37.68
ATOM	4107	O	ASP	735	46.447	3.178	31.579	1.00	36.83
ATOM	4108	N	CYS	736	46.996	1.967	29.734	1.00	35.06
ATOM	4109	CA	CYS	736	47.858	2.979	29.140	1.00	32.91
ATOM	4110	CB	CYS	736	48.499	2.469	27.848	1.00	27.65
ATOM	4111	SG	CYS	736	49.631	1.067	27.989	1.00	31.08
ATOM	4112	C	CYS	736	47.054	4.232	28.828	1.00	35.28
ATOM	4113	O	CYS	736	47.595	5.334	28.810	1.00	35.52
ATOM	4114	N	TRP	737	45.742	4.078	28.677	1.00	38.73
ATOM	4115	CA	TRP	737	44.885	5.217	28.352	1.00	41.10
ATOM	4116	CB	TRP	737	43.890	4.816	27.266	1.00	41.22
ATOM	4117	CG	TRP	737	44.535	4.362	25.994	1.00	40.65
ATOM	4118	CD2	TRP	737	43.976	3.465	25.026	1.00	41.90
ATOM	4119	CE2	TRP	737	44.932	3.325	23.990	1.00	41.02
ATOM	4120	CE3	TRP	737	42.763	2.764	24.930	1.00	40.44
ATOM	4121	CD1	TRP	737	45.766	4.721	25.517	1.00	39.14
ATOM	4122	NE1	TRP	737	46.011	4.103	24.316	1.00	37.93
ATOM	4123	CZ2	TRP	737	44.708	2.512	22.875	1.00	40.92
ATOM	4124	CZ3	TRP	737	42.549	1.956	23.820	1.00	38.42
ATOM	4125	CH2	TRP	737	43.518	1.837	22.812	1.00	36.49
ATOM	4126	C	TRP	737	44.159	5.847	29.538	1.00	41.39
ATOM	4127	O	TRP	737	43.163	6.551	29.366	1.00	40.86
ATOM	4128	N	HIS	738	44.685	5.643	30.743	1.00	43.61
ATOM	4129	CA	HIS	738	44.059	6.197	31.941	1.00	44.35
ATOM	4130	CB	HIS	738	44.698	5.596	33.183	1.00	45.31
ATOM	4131	CG	HIS	738	43.970	5.922	34.446	1.00	50.87
ATOM	4132	CD2	HIS	738	43.685	7.111	35.026	1.00	49.13
ATOM	4133	ND1	HIS	738	43.401	4.961	35.252	1.00	52.48
ATOM	4134	CE1	HIS	738	42.798	5.541	36.275	1.00	55.70
ATOM	4135	NE2	HIS	738	42.955	6.848	36.159	1.00	51.42
ATOM	4136	C	HIS	738	44.202	7.714	31.969	1.00	44.15
ATOM	4137	O	HIS	738	45.294	8.223	31.787	1.00	43.14
ATOM	4138	N	ALA	739	43.115	8.428	32.272	1.00	45.42
ATOM	4139	CA	ALA	739	43.141	9.895	32.318	1.00	47.29
ATOM	4140	CB	ALA	739	41.792	10.426	32.752	1.00	49.75
ATOM	4141	C	ALA	739	44.240	10.454	33.223	1.00	48.73
ATOM	4142	O	ALA	739	44.921	11.415	32.868	1.00	49.32
ATOM	4143	N	VAL	740	44.331	9.893	34.425	1.00	50.51
ATOM	4144	CA	VAL	740	45.332	10.262	35.424	1.00	51.32
ATOM	4145	CB	VAL	740	44.861	9.880	36.842	1.00	52.29
ATOM	4146	CG1	VAL	740	45.905	10.254	37.869	1.00	53.73
ATOM	4147	CG2	VAL	740	43.551	10.575	37.152	1.00	53.54
ATOM	4148	C	VAL	740	46.656	9.535	35.121	1.00	51.06
ATOM	4149	O	VAL	740	46.780	8.320	35.348	1.00	50.81
ATOM	4150	N	PRO	741	47.670	10.280	34.657	1.00	50.12
ATOM	4151	CD	PRO	741	47.595	11.738	34.454	1.00	50.19
ATOM	4152	CA	PRO	741	49.003	9.775	34.294	1.00	51.10
ATOM	4153	CB	PRO	741	49.790	11.060	34.024	1.00	50.35
ATOM	4154	CG	PRO	741	48.731	11.978	33.492	1.00	50.13

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ATOM	4155	C	PRO	741	49.687	8.902	35.340	1.00	52.02
ATOM	4156	O	PRO	741	50.374	7.941	34.998	1.00	50.79
ATOM	4157	N	SER	742	49.482	9.228	36.613	1.00	53.75
ATOM	4158	CA	SER	742	50.079	8.474	37.708	1.00	54.58
ATOM	4159	CB	SER	742	49.921	9.245	39.020	1.00	57.25
ATOM	4160	OG	SER	742	48.572	9.629	39.237	1.00	61.69
ATOM	4161	C	SER	742	49.479	7.077	37.851	1.00	53.33
ATOM	4162	O	SER	742	50.074	6.189	38.464	1.00	52.98
ATOM	4163	N	GLN	743	48.286	6.897	37.305	1.00	52.97
ATOM	4164	CA	GLN	743	47.616	5.613	37.390	1.00	52.15
ATOM	4165	CB	GLN	743	46.108	5.827	37.505	1.00	56.12
ATOM	4166	CG	GLN	743	45.506	5.374	38.838	1.00	60.50
ATOM	4167	CD	GLN	743	46.269	5.887	40.046	1.00	64.45
ATOM	4168	OE1	GLN	743	46.910	5.114	40.752	1.00	65.64
ATOM	4169	NE2	GLN	743	46.199	7.194	40.290	1.00	67.99
ATOM	4170	C	GLN	743	47.963	4.690	36.229	1.00	49.54
ATOM	4171	O	GLN	743	47.629	3.499	36.246	1.00	50.07
ATOM	4172	N	ARG	744	48.605	5.241	35.202	1.00	46.93
ATOM	4173	CA	ARG	744	49.010	4.437	34.044	1.00	44.51
ATOM	4174	CB	ARG	744	49.478	5.330	32.894	1.00	39.30
ATOM	4175	CG	ARG	744	48.433	6.300	32.360	1.00	32.53
ATOM	4176	CD	ARG	744	48.991	7.178	31.254	1.00	25.50
ATOM	4177	NE	ARG	744	48.034	8.218	30.932	1.00	32.16
ATOM	4178	CZ	ARG	744	48.352	9.454	30.542	1.00	34.35
ATOM	4179	NH1	ARG	744	49.622	9.814	30.400	1.00	30.49
ATOM	4180	NH2	ARG	744	47.382	10.349	30.350	1.00	32.23
ATOM	4181	C	ARG	744	50.153	3.498	34.472	1.00	44.61
ATOM	4182	O	ARG	744	50.833	3.741	35.474	1.00	47.68
ATOM	4183	N	PRO	745	50.319	2.365	33.765	1.00	43.21
ATOM	4184	CD	PRO	745	49.444	1.737	32.763	1.00	42.00
ATOM	4185	CA	PRO	745	51.414	1.470	34.157	1.00	40.11
ATOM	4186	CB	PRO	745	51.004	0.132	33.532	1.00	37.54
ATOM	4187	CG	PRO	745	50.251	0.515	32.335	1.00	36.49
ATOM	4188	C	PRO	745	52.744	1.956	33.612	1.00	39.15
ATOM	4189	O	PRO	745	52.807	2.654	32.602	1.00	40.56
ATOM	4190	N	THR	746	53.812	1.626	34.316	1.00	37.77
ATOM	4191	CA	THR	746	55.135	2.020	33.886	1.00	37.61
ATOM	4192	CB	THR	746	56.113	2.132	35.091	1.00	39.14
ATOM	4193	OG1	THR	746	56.439	0.824	35.600	1.00	35.16
ATOM	4194	CG2	THR	746	55.489	2.990	36.195	1.00	36.82
ATOM	4195	C	THR	746	55.687	1.036	32.852	1.00	36.75
ATOM	4196	O	THR	746	55.228	-0.103	32.772	1.00	32.89
ATOM	4197	N	PHE	747	56.649	1.482	32.043	1.00	36.56
ATOM	4198	CA	PHE	747	57.267	0.599	31.055	1.00	33.79
ATOM	4199	CB	PHE	747	58.305	1.350	30.226	1.00	28.85
ATOM	4200	CG	PHE	747	57.702	2.123	29.103	1.00	30.71
ATOM	4201	CD1	PHE	747	57.060	1.455	28.059	1.00	26.42
ATOM	4202	CD2	PHE	747	57.749	3.510	29.080	1.00	28.73
ATOM	4203	CE1	PHE	747	56.469	2.154	27.025	1.00	26.56
ATOM	4204	CE2	PHE	747	57.150	4.216	28.047	1.00	28.97
ATOM	4205	CZ	PHE	747	56.518	3.535	27.018	1.00	28.95
ATOM	4206	C	PHE	747	57.901	-0.593	31.732	1.00	34.64

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ATOM	4207	O	PHE	747	58.008	-1.667	31.156	1.00	31.47
ATOM	4208	N	LYS	748	58.328	-0.399	32.972	1.00	38.86
ATOM	4209	CA	LYS	748	58.920	-1.480	33.727	1.00	39.79
ATOM	4210	CB	LYS	748	59.529	-0.952	35.026	1.00	43.68
ATOM	4211	CG	LYS	748	60.200	-2.047	35.838	1.00	48.11
ATOM	4212	CD	LYS	748	60.917	-1.515	37.064	1.00	51.33
ATOM	4213	CE	LYS	748	61.353	-2.660	37.973	1.00	51.17
ATOM	4214	NZ	LYS	748	62.135	-2.141	39.127	1.00	56.55
ATOM	4215	C	LYS	748	57.813	-2.503	34.008	1.00	41.14
ATOM	4216	O	LYS	748	58.025	-3.706	33.848	1.00	38.24
ATOM	4217	N	GLN	749	56.622	-2.008	34.383	1.00	41.20
ATOM	4218	CA	GLN	749	55.454	-2.856	34.669	1.00	40.49
ATOM	4219	CB	GLN	749	54.254	-2.015	35.134	1.00	45.70
ATOM	4220	CG	GLN	749	54.378	-1.368	36.500	1.00	50.61
ATOM	4221	CD	GLN	749	53.203	-0.441	36.797	1.00	55.26
ATOM	4222	OE1	GLN	749	53.392	0.727	37.123	1.00	58.00
ATOM	4223	NE2	GLN	749	51.988	-0.951	36.665	1.00	59.25
ATOM	4224	C	GLN	749	55.049	-3.588	33.397	1.00	37.42
ATOM	4225	O	GLN	749	54.964	-4.810	33.369	1.00	36.00
ATOM	4226	N	LEU	750	54.810	-2.817	32.340	1.00	36.76
ATOM	4227	CA	LEU	750	54.409	-3.355	31.033	1.00	35.39
ATOM	4228	CB	LEU	750	54.358	-2.241	29.984	1.00	30.97
ATOM	4229	CG	LEU	750	53.369	-1.091	30.177	1.00	27.36
ATOM	4230	CD1	LEU	750	53.745	0.037	29.217	1.00	29.15
ATOM	4231	CD2	LEU	750	51.941	-1.578	29.934	1.00	29.22
ATOM	4232	C	LEU	750	55.369	-4.437	30.557	1.00	35.16
ATOM	4233	O	LEU	750	54.934	-5.449	30.014	1.00	34.45
ATOM	4234	N	VAL	751	56.673	-4.212	30.721	1.00	38.76
ATOM	4235	CA	VAL	751	57.656	-5.217	30.312	1.00	38.69
ATOM	4236	CB	VAL	751	59.129	-4.724	30.485	1.00	33.81
ATOM	4237	CG1	VAL	751	60.092	-5.836	30.120	1.00	32.04
ATOM	4238	CG2	VAL	751	59.415	-3.535	29.598	1.00	30.67
ATOM	4239	C	VAL	751	57.428	-6.493	31.131	1.00	41.68
ATOM	4240	O	VAL	751	57.492	-7.599	30.594	1.00	39.92
ATOM	4241	N	GLU	752	57.109	-6.338	32.414	1.00	44.22
ATOM	4242	CA	GLU	752	56.854	-7.501	33.266	1.00	47.43
ATOM	4243	CB	GLU	752	56.779	-7.078	34.743	1.00	49.29
ATOM	4244	CG	GLU	752	58.093	-6.448	35.212	1.00	53.53
ATOM	4245	CD	GLU	752	58.215	-6.249	36.707	1.00	53.05
ATOM	4246	OE1	GLU	752	58.554	-5.123	37.136	1.00	53.63
ATOM	4247	OE2	GLU	752	58.021	-7.228	37.452	1.00	56.18
ATOM	4248	C	GLU	752	55.594	-8.256	32.809	1.00	46.90
ATOM	4249	O	GLU	752	55.646	-9.464	32.551	1.00	43.85
ATOM	4250	N	ASP	753	54.490	-7.529	32.640	1.00	48.05
ATOM	4251	CA	ASP	753	53.232	-8.128	32.193	1.00	48.46
ATOM	4252	CB	ASP	753	52.119	-7.090	32.118	1.00	51.25
ATOM	4253	CG	ASP	753	51.579	-6.707	33.467	1.00	54.20
ATOM	4254	OD1	ASP	753	51.440	-7.589	34.330	1.00	57.31
ATOM	4255	OD2	ASP	753	51.281	-5.513	33.659	1.00	55.58
ATOM	4256	C	ASP	753	53.371	-8.771	30.837	1.00	48.59
ATOM	4257	O	ASP	753	53.001	-9.930	30.649	1.00	49.69
ATOM	4258	N	LEU	754	53.903	-8.009	29.889	1.00	47.21

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ATOM	4259	CA	LEU	754	54.102	-8.489	28.523	1.00	46.37
ATOM	4260	CB	LEU	754	54.664	-7.385	27.625	1.00	44.16
ATOM	4261	CG	LEU	754	53.621	-6.366	27.152	1.00	46.35
ATOM	4262	CD1	LEU	754	54.296	-5.272	26.343	1.00	45.11
ATOM	4263	CD2	LEU	754	52.514	-7.070	26.349	1.00	42.89
ATOM	4264	C	LEU	754	55.004	-9.703	28.481	1.00	47.08
ATOM	4265	O	LEU	754	54.818	-10.590	27.659	1.00	45.02
ATOM	4266	N	ASP	755	55.969	-9.755	29.385	1.00	49.68
ATOM	4267	CA	ASP	755	56.890	-10.876	29.487	1.00	51.62
ATOM	4268	CB	ASP	755	57.883	-10.586	30.615	1.00	54.90
ATOM	4269	CG	ASP	755	59.009	-11.589	30.702	1.00	59.00
ATOM	4270	OD1	ASP	755	59.694	-11.608	31.746	1.00	63.70
ATOM	4271	OD2	ASP	755	59.223	-12.346	29.728	1.00	60.31
ATOM	4272	C	ASP	755	56.059	-12.117	29.817	1.00	51.50
ATOM	4273	O	ASP	755	56.119	-13.150	29.138	1.00	47.11
ATOM	4274	N	ARG	756	55.237	-11.958	30.844	1.00	51.81
ATOM	4275	CA	ARG	756	54.362	-13.009	31.328	1.00	51.44
ATOM	4276	CB	ARG	756	53.635	-12.519	32.582	1.00	54.52
ATOM	4277	CG	ARG	756	52.459	-13.358	33.027	1.00	55.00
ATOM	4278	CD	ARG	756	51.815	-12.727	34.255	1.00	59.54
ATOM	4279	NE	ARG	756	51.417	-11.335	34.026	1.00	64.01
ATOM	4280	CZ	ARG	756	50.366	-10.960	33.301	1.00	65.76
ATOM	4281	NH1	ARG	756	49.598	-11.866	32.721	1.00	63.56
ATOM	4282	NH2	ARG	756	50.061	-9.676	33.183	1.00	66.59
ATOM	4283	C	ARG	756	53.361	-13.440	30.260	1.00	50.03
ATOM	4284	O	ARG	756	53.267	-14.622	29.960	1.00	49.98
ATOM	4285	N	ILE	757	52.645	-12.483	29.673	1.00	46.87
ATOM	4286	CA	ILE	757	51.656	-12.789	28.644	1.00	44.28
ATOM	4287	CB	ILE	757	50.919	-11.532	28.125	1.00	40.46
ATOM	4288	CG2	ILE	757	49.923	-11.923	27.062	1.00	38.44
ATOM	4289	CG1	ILE	757	50.202	-10.830	29.277	1.00	39.74
ATOM	4290	CD1	ILE	757	49.481	-9.551	28.920	1.00	40.68
ATOM	4291	C	ILE	757	52.251	-13.528	27.454	1.00	44.20
ATOM	4292	O	ILE	757	51.643	-14.469	26.959	1.00	40.28
ATOM	4293	N	VAL	758	53.440	-13.111	27.014	1.00	47.56
ATOM	4294	CA	VAL	758	54.102	-13.745	25.874	1.00	48.90
ATOM	4295	CB	VAL	758	55.543	-13.177	25.609	1.00	47.01
ATOM	4296	CG1	VAL	758	56.198	-13.920	24.456	1.00	44.38
ATOM	4297	CG2	VAL	758	55.493	-11.714	25.262	1.00	47.85
ATOM	4298	C	VAL	758	54.249	-15.232	26.149	1.00	51.79
ATOM	4299	O	VAL	758	54.043	-16.055	25.258	1.00	49.80
ATOM	4300	N	ALA	759	54.622	-15.550	27.386	1.00	54.80
ATOM	4301	CA	ALA	759	54.825	-16.925	27.814	1.00	57.15
ATOM	4302	CB	ALA	759	55.406	-16.948	29.212	1.00	56.77
ATOM	4303	C	ALA	759	53.524	-17.717	27.777	1.00	60.83
ATOM	4304	O	ALA	759	53.487	-18.849	27.296	1.00	63.59
ATOM	4305	N	LEU	760	52.452	-17.112	28.271	1.00	61.74
ATOM	4306	CA	LEU	760	51.151	-17.760	28.295	1.00	61.29
ATOM	4307	CB	LEU	760	50.280	-17.149	29.388	1.00	60.41
ATOM	4308	CG	LEU	760	50.808	-17.323	30.812	1.00	58.68
ATOM	4309	CD1	LEU	760	49.917	-16.603	31.815	1.00	59.64
ATOM	4310	CD2	LEU	760	50.899	-18.799	31.138	1.00	57.84

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ATOM	4311	C	LEU	760	50.439	-17.706	26.951	1.00	63.42
ATOM	4312	O	LEU	760	49.282	-18.121	26.842	1.00	63.68
ATOM	4313	N	THR	761	51.113	-17.200	25.924	1.00	66.71
ATOM	4314	CA	THR	761	50.512	-17.109	24.586	1.00	68.48
ATOM	4315	CB	THR	761	50.794	-15.734	23.922	1.00	68.21
ATOM	4316	OG1	THR	761	50.193	-14.695	24.701	1.00	70.34
ATOM	4317	CG2	THR	761	50.202	-15.684	22.530	1.00	64.45
ATOM	4318	C	THR	761	51.030	-18.225	23.688	1.00	69.65
ATOM	4319	O	THR	761	52.230	-18.492	23.623	1.00	70.43
ATOM	4320	SG	CYS	1603	18.668	-9.074	20.131	0.50	30.57
ATOM	4321	CG	MET	534	69.414	12.079	23.224	0.50	36.86
ATOM	4322	SD	MET	534	69.162	13.149	24.646	0.50	40.20
ATOM	4323	CE	MET	534	70.204	12.299	25.912	0.50	41.95
ATOM	4324	SG	CYS	603	56.218	-8.072	16.341	0.50	37.35
ATOM	4325	OH2	TIP	1	71.863	25.340	2.719	1.00	24.40
ATOM	4326	OH2	TIP	2	39.671	4.177	15.837	1.00	36.87
ATOM	4327	OH2	TIP	3	83.765	19.802	10.549	1.00	26.81
ATOM	4328	OH2	TIP	4	83.844	20.193	7.757	1.00	30.07
ATOM	4329	OH2	TIP	5	75.192	16.430	6.693	1.00	26.76
ATOM	4330	OH2	TIP	6	86.579	19.662	9.323	1.00	36.11
ATOM	4331	OH2	TIP	7	52.204	10.911	24.392	1.00	36.83
ATOM	4332	OH2	TIP	8	55.174	9.435	22.514	1.00	21.93
ATOM	4333	OH2	TIP	9	57.077	4.556	32.580	1.00	25.17
ATOM	4334	OH2	TIP	10	52.281	4.737	13.300	1.00	20.79
ATOM	4335	OH2	TIP	11	41.402	5.304	22.893	1.00	39.17
ATOM	4336	OH2	TIP	12	45.088	8.857	21.604	1.00	35.14
ATOM	4337	OH2	TIP	13	64.519	-2.772	28.799	1.00	47.52
ATOM	4338	OH2	TIP	14	77.327	12.960	23.832	1.00	34.47
ATOM	4339	OH2	TIP	15	79.366	17.021	18.247	1.00	47.49
ATOM	4340	OH2	TIP	16	83.087	11.573	15.986	1.00	22.80
ATOM	4341	OH2	TIP	17	13.977	-9.804	0.222	1.00	24.88
ATOM	4342	OH2	TIP	18	38.451	0.155	5.081	1.00	41.03
ATOM	4343	OH2	TIP	20	27.109	6.286	4.902	1.00	27.69
ATOM	4344	OH2	TIP	21	34.379	-1.750	16.771	1.00	47.69
ATOM	4345	OH2	TIP	22	20.394	2.449	27.821	1.00	54.32
ATOM	4346	OH2	TIP	23	50.587	-11.642	38.062	1.00	45.31
ATOM	4347	OH2	TIP	24	17.137	-5.949	-1.716	1.00	27.63
ATOM	4348	OH2	TIP	25	27.604	7.961	15.119	1.00	47.19
ATOM	4349	OH2	TIP	26	31.446	0.136	6.605	1.00	29.98
ATOM	4350	OH2	TIP	27	27.030	-13.047	27.803	1.00	28.86
ATOM	4351	OH2	TIP	28	28.477	-17.191	13.067	1.00	37.44
ATOM	4352	OH2	TIP	29	88.748	14.279	8.091	1.00	32.72
ATOM	4353	OH2	TIP	30	-2.392	-3.684	11.343	1.00	41.86
ATOM	4354	OH2	TIP	31	34.968	-4.221	18.549	1.00	40.51
ATOM	4355	OH2	TIP	32	80.581	17.982	9.655	1.00	27.85
ATOM	4356	OH2	TIP	33	5.522	3.773	10.805	1.00	24.60
ATOM	4357	OH2	TIP	34	-10.747	5.416	11.174	1.00	29.27
ATOM	4358	OH2	TIP	35	29.049	-8.816	19.978	1.00	35.24
ATOM	4359	OH2	TIP	36	5.871	3.463	13.481	1.00	26.62
ATOM	4360	OH2	TIP	37	31.834	2.899	0.207	1.00	49.70
ATOM	4361	OH2	TIP	38	19.799	2.012	-3.941	1.00	29.67
ATOM	4362	OH2	TIP	39	62.060	2.679	32.659	1.00	54.86

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ATOM	4363	OH2	TIP	40	21.100	-6.883	-4.054	1.00	22.33
ATOM	4364	OH2	TIP	41	-15.675	8.744	22.559	1.00	44.54
ATOM	4365	OH2	TIP	42	40.066	2.225	8.567	1.00	57.00
ATOM	4366	OH2	TIP	43	19.477	11.293	-0.049	1.00	37.77
ATOM	4367	OH2	TIP	44	67.060	9.047	17.334	1.00	25.14
ATOM	4368	OH2	TIP	45	87.829	18.937	18.529	1.00	45.92
ATOM	4369	OH2	TIP	46	74.741	16.956	3.987	1.00	40.33
ATOM	4370	OH2	TIP	47	29.411	16.888	10.525	1.00	38.41
ATOM	4371	OH2	TIP	48	66.592	7.020	15.108	1.00	36.15
ATOM	4372	OH2	TIP	49	85.071	21.432	5.755	1.00	19.89
ATOM	4373	OH2	TIP	50	-4.842	3.281	3.118	1.00	28.22
ATOM	4374	OH2	TIP	51	19.454	5.250	4.876	1.00	34.86
ATOM	4375	OH2	TIP	53	34.785	5.433	24.743	1.00	30.40
ATOM	4376	OH2	TIP	54	34.792	-17.150	13.665	1.00	35.81
ATOM	4377	OH2	TIP	55	59.956	7.380	27.941	1.00	36.76
ATOM	4378	OH2	TIP	56	-7.327	-1.518	6.428	1.00	39.13
ATOM	4379	OH2	TIP	57	55.164	12.120	25.338	1.00	38.87
ATOM	4380	OH2	TIP	58	68.637	6.832	16.698	1.00	54.96
ATOM	4381	OH2	TIP	59	73.778	20.869	19.031	1.00	35.01
ATOM	4382	OH2	TIP	60	3.582	-8.363	-8.103	1.00	16.71
ATOM	4383	OH2	TIP	61	38.051	10.933	5.487	1.00	32.85
ATOM	4384	OH2	TIP	62	29.727	-9.630	-1.370	1.00	30.92
ATOM	4385	OH2	TIP	64	49.186	1.253	12.066	1.00	42.67
ATOM	4386	OH2	TIP	65	41.375	3.989	28.951	1.00	37.95
ATOM	4387	OH2	TIP	66	10.798	-13.119	1.125	1.00	38.26
ATOM	4388	OH2	TIP	67	-1.079	-4.386	21.428	1.00	27.92
ATOM	4389	OH2	TIP	68	30.327	16.346	13.295	1.00	53.21
ATOM	4390	OH2	TIP	69	8.319	4.437	3.449	1.00	23.63
ATOM	4391	OH2	TIP	70	73.152	18.809	22.631	1.00	36.45
ATOM	4392	OH2	TIP	71	-7.984	-3.476	25.048	1.00	33.16
ATOM	4393	OH2	TIP	72	66.529	-4.720	28.421	1.00	66.32
ATOM	4394	OH2	TIP	73	21.577	-20.723	4.868	1.00	48.14
ATOM	4395	OH2	TIP	74	59.417	-6.760	4.957	1.00	48.73
ATOM	4396	OH2	TIP	75	16.509	-13.306	-2.942	1.00	41.02
ATOM	4397	OH2	TIP	76	-15.064	7.473	4.275	1.00	26.77
ATOM	4398	OH2	TIP	77	33.118	2.917	13.384	1.00	41.38
ATOM	4399	OH2	TIP	78	0.112	-2.913	10.809	1.00	27.49
ATOM	4400	OH2	TIP	79	17.448	2.562	5.507	1.00	16.32
ATOM	4401	OH2	TIP	81	27.445	3.796	6.134	1.00	29.83
ATOM	4402	OH2	TIP	82	-8.708	6.231	9.598	1.00	27.66
ATOM	4403	OH2	TIP	83	1.565	-1.998	8.758	1.00	33.46
ATOM	4404	OH2	TIP	84	-4.774	-3.153	7.049	1.00	36.59
ATOM	4405	OH2	TIP	85	17.443	3.105	1.795	1.00	20.39
ATOM	4406	OH2	TIP	86	20.120	3.387	2.918	1.00	30.35
ATOM	4407	OH2	TIP	87	0.466	-2.238	22.190	1.00	20.30
ATOM	4408	OH2	TIP	88	19.749	-6.018	-1.687	1.00	21.33
ATOM	4409	OH2	TIP	89	10.505	-15.695	6.861	1.00	38.80
ATOM	4410	OH2	TIP	90	4.223	-12.113	11.774	1.00	34.18
ATOM	4411	OH2	TIP	91	6.297	1.090	-3.192	1.00	24.40
ATOM	4412	OH2	TIP	92	-13.540	1.554	5.413	1.00	34.94
ATOM	4413	OH2	TIP	93	15.607	-7.315	0.017	1.00	26.30
ATOM	4414	OH2	TIP	94	-1.868	-5.461	3.839	1.00	37.12

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ATOM	4415	OH2	TIP	95	12.718	5.095	-4.401	1.00	40.61
ATOM	4416	OH2	TIP	96	69.849	27.233	2.056	1.00	41.42
ATOM	4417	OH2	TIP	97	24.374	-13.311	0.143	1.00	52.75
ATOM	4418	OH2	TIP	98	60.424	-4.582	34.237	1.00	42.02
ATOM	4419	OH2	TIP	99	10.589	5.757	3.485	1.00	61.53
ATOM	4420	OH2	TIP	100	-9.564	-3.999	4.718	1.00	29.02
ATOM	4421	OH2	TIP	101	73.085	-1.967	10.565	1.00	59.23
ATOM	4422	OH2	TIP	102	-3.172	5.701	30.623	1.00	30.51
ATOM	4423	OH2	TIP	103	36.672	0.620	11.780	1.00	53.77
ATOM	4424	OH2	TIP	104	21.408	6.462	16.955	1.00	27.62
ATOM	4425	OH2	TIP	105	31.224	0.791	19.345	1.00	77.65
ATOM	4426	OH2	TIP	106	5.660	-8.451	22.197	1.00	49.50
ATOM	4427	OH2	TIP	107	-12.988	8.471	17.441	1.00	31.69
ATOM	4428	OH2	TIP	108	26.733	-10.524	-0.894	1.00	25.26
ATOM	4429	OH2	TIP	109	24.182	2.026	18.156	1.00	35.87
ATOM	4430	OH2	TIP	110	-1.822	12.848	3.561	1.00	35.44
ATOM	4431	OH2	TIP	111	59.584	13.491	33.225	1.00	40.47
ATOM	4432	OH2	TIP	112	4.402	-10.813	1.929	1.00	47.07
ATOM	4433	OH2	TIP	113	8.032	2.916	0.940	1.00	40.79
ATOM	4434	OH2	TIP	114	75.905	1.522	25.912	1.00	55.51
ATOM	4435	OH2	TIP	115	48.960	15.737	14.249	1.00	38.97
ATOM	4436	OH2	TIP	116	2.333	-11.271	9.174	1.00	29.12
ATOM	4437	OH2	TIP	117	83.062	26.404	12.925	1.00	41.17
ATOM	4438	OH2	TIP	118	8.816	-6.440	-3.424	1.00	48.26
ATOM	4439	OH2	TIP	119	-8.594	4.575	4.258	1.00	32.68
ATOM	4440	OH2	TIP	120	7.695	-13.769	8.481	1.00	39.22
ATOM	4441	OH2	TIP	121	51.500	6.285	10.369	1.00	25.18
ATOM	4442	OH2	TIP	122	20.720	3.849	15.625	1.00	22.46
ATOM	4443	OH2	TIP	123	73.111	3.718	20.617	1.00	28.26
ATOM	4444	OH2	TIP	124	5.312	-11.608	22.516	1.00	32.74
ATOM	4445	OH2	TIP	125	34.207	2.437	16.601	1.00	65.04
ATOM	4446	OH2	TIP	126	9.535	-11.998	7.085	1.00	25.13
ATOM	4447	OH2	TIP	127	8.227	3.912	-1.495	1.00	43.73
ATOM	4448	OH2	TIP	129	7.312	7.072	2.922	1.00	47.65
ATOM	4449	OH2	TIP	130	35.824	-1.660	0.135	1.00	30.43
ATOM	4450	OH2	TIP	131	44.723	10.285	11.144	1.00	32.74
ATOM	4451	OH2	TIP	132	27.941	-13.172	18.733	1.00	58.65
ATOM	4452	OH2	TIP	133	45.301	11.497	21.408	1.00	35.00
ATOM	4453	OH2	TIP	134	57.705	-10.824	14.202	1.00	69.18
ATOM	4454	OH2	TIP	135	-3.108	15.385	16.685	1.00	38.07
ATOM	4455	OH2	TIP	136	85.884	11.182	9.044	1.00	32.04
ATOM	4456	OH2	TIP	137	12.840	-2.444	1.983	1.00	30.08
ATOM	4457	OH2	TIP	138	75.645	3.496	20.607	1.00	33.94
ATOM	4458	OH2	TIP	139	13.020	7.518	-2.510	1.00	40.68
ATOM	4459	OH2	TIP	140	11.245	-10.070	0.729	1.00	26.02
ATOM	4460	OH2	TIP	141	59.563	10.829	14.466	1.00	71.34
ATOM	4461	OH2	TIP	142	13.671	-16.214	3.489	1.00	39.47
ATOM	4462	OH2	TIP	143	-6.358	-3.421	16.520	1.00	37.08
ATOM	4463	OH2	TIP	144	25.629	-12.764	3.534	1.00	50.51
ATOM	4464	OH2	TIP	145	-16.459	10.869	6.524	1.00	38.40
ATOM	4465	OH2	TIP	146	86.598	12.840	7.028	1.00	47.80
ATOM	4466	OH2	TIP	147	32.139	-4.674	1.757	1.00	32.43

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ATOM	4467	OH2	TIP	148	44.890	7.505	11.806	1.00	32.46
ATOM	4468	OH2	TIP	149	80.781	12.432	16.562	1.00	47.77
ATOM	4469	OH2	TIP	150	3.017	-7.101	-1.917	1.00	40.92
ATOM	4470	OH2	TIP	151	31.784	-6.139	20.968	1.00	38.23
ATOM	4471	OH2	TIP	152	74.835	-2.597	12.290	1.00	48.89
ATOM	4472	OH2	TIP	153	7.509	6.768	-1.083	1.00	46.02
ATOM	4473	OH2	TIP	154	71.732	5.360	21.908	1.00	33.30
ATOM	4474	OH2	TIP	155	68.150	-5.075	8.794	1.00	39.31
ATOM	4475	OH2	TIP	156	0.148	-9.544	6.872	1.00	41.37
ATOM	4476	OH2	TIP	157	67.878	18.204	10.861	1.00	51.19
ATOM	4477	OH2	TIP	158	3.652	8.829	4.428	1.00	31.24
ATOM	4478	OH2	TIP	159	52.100	11.362	18.433	1.00	40.73
ATOM	4479	OH2	TIP	161	-10.357	6.783	4.861	1.00	35.13
ATOM	4480	OH2	TIP	162	76.471	1.562	-0.853	1.00	59.17
ATOM	4481	OH2	TIP	163	10.073	-12.056	17.071	1.00	44.69
ATOM	4482	OH2	TIP	164	34.163	14.271	18.254	1.00	39.59
ATOM	4483	OH2	TIP	165	2.320	-7.990	16.820	1.00	38.19
ATOM	4484	OH2	TIP	166	29.696	1.908	6.098	1.00	38.02
ATOM	4485	OH2	TIP	167	32.626	-17.410	11.766	1.00	48.15
ATOM	4486	OH2	TIP	168	42.244	18.049	11.043	1.00	50.95
ATOM	4487	OH2	TIP	169	87.907	10.574	5.721	1.00	60.28
ATOM	4488	OH2	TIP	170	70.313	-3.998	25.141	1.00	72.64
ATOM	4489	OH2	TIP	171	77.603	5.679	23.952	1.00	43.23
ATOM	4490	OH2	TIP	172	-0.942	-8.153	4.508	1.00	55.10
ATOM	4491	OH2	TIP	173	34.297	15.574	1.690	1.00	34.19
ATOM	4492	OH2	TIP	174	-9.643	7.829	7.414	1.00	50.48
ATOM	4493	OH2	TIP	175	11.618	5.655	7.455	1.00	43.37
ATOM	4494	OH2	TIP	176	-8.705	13.841	13.642	1.00	72.49
ATOM	4495	OH2	TIP	177	32.009	3.416	18.257	1.00	44.16
ATOM	4496	OH2	TIP	178	-8.651	10.180	24.352	1.00	44.85
ATOM	4497	OH2	TIP	179	-1.153	-6.532	15.548	1.00	32.90
ATOM	4498	OH2	TIP	180	80.235	0.749	15.508	1.00	34.75
ATOM	4499	OH2	TIP	181	67.222	20.490	-1.574	1.00	40.76
ATOM	4500	OH2	TIP	182	-0.471	4.367	1.248	1.00	36.58
ATOM	4501	OH2	TIP	183	0.149	6.517	2.578	1.00	40.12
ATOM	4502	OH2	TIP	184	-1.186	8.867	1.311	1.00	44.77
ATOM	4503	OH2	TIP	185	-5.093	9.260	2.252	1.00	52.07
ATOM	4504	OH2	TIP	186	-7.235	10.227	3.913	1.00	58.53
ATOM	4505	OH2	TIP	187	2.724	7.169	0.879	1.00	47.77
ATOM	4506	OH2	TIP	188	5.527	11.031	8.519	1.00	34.40
ATOM	4507	OH2	TIP	189	63.927	12.721	22.689	1.00	40.75
ATOM	4508	OH2	TIP	190	79.264	1.066	18.321	1.00	41.34
ATOM	4509	OH2	TIP	191	59.247	-11.825	7.256	1.00	79.86
ATOM	4510	OH2	TIP	192	13.994	-0.972	-4.310	1.00	31.15
ATOM	4511	OH2	TIP	193	59.546	3.024	33.227	1.00	40.34
ATOM	4512	OH2	TIP	194	32.179	13.637	19.964	1.00	48.25
ATOM	4513	OH2	TIP	195	72.178	16.188	22.879	1.00	42.72
ATOM	4514	OH2	TIP	196	0.898	-8.663	14.348	1.00	41.76
ATOM	4515	OH2	TIP	197	-0.490	5.455	30.574	1.00	38.30
ATOM	4516	OH2	TIP	199	-1.277	-4.244	27.691	1.00	56.27
ATOM	4517	OH2	TIP	200	81.605	15.360	17.272	1.00	42.05
ATOM	4518	OH2	TIP	201	-17.534	4.081	23.779	1.00	59.65

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ATOM	4519	OH2 TIP	202	27.748	10.634	14.595	1.00	49.97
ATOM	4520	OH2 TIP	203	34.891	4.468	27.604	1.00	60.26
ATOM	4521	OH2 TIP	204	-3.460	-4.448	9.045	1.00	44.70
ATOM	4522	OH2 TIP	205	42.705	7.590	22.526	1.00	35.77
ATOM	4523	OH2 TIP	206	52.983	11.950	21.969	1.00	35.12
ATOM	4524	OH2 TIP	207	26.871	14.098	19.820	1.00	53.04
ATOM	4525	OH2 TIP	208	-7.184	9.323	6.370	1.00	37.49
ATOM	4526	OH2 TIP	209	86.676	5.553	15.911	1.00	72.92
ATOM	4527	OH2 TIP	210	55.080	15.928	20.414	1.00	68.75
ATOM	4528	OH2 TIP	211	51.512	19.264	22.672	1.00	54.72
ATOM	4529	OH2 TIP	212	19.988	7.127	6.976	1.00	45.55
ATOM	4530	OH2 TIP	213	28.905	2.021	-3.430	1.00	48.55
ATOM	4531	OH2 TIP	214	26.446	2.593	-4.753	1.00	55.04
ATOM	4532	OH2 TIP	215	36.539	2.911	18.446	1.00	38.50
ATOM	4533	OH2 TIP	216	16.807	-20.725	14.119	1.00	56.03
ATOM	4534	OH2 TIP	217	28.203	-14.485	6.172	1.00	62.90
ATOM	4535	OH2 TIP	218	31.519	1.503	-2.010	1.00	56.19
ATOM	4536	OH2 TIP	219	10.014	-16.571	15.451	1.00	46.37
ATOM	4537	OH2 TIP	220	7.126	-11.922	5.526	1.00	56.89
ATOM	4538	OH2 TIP	221	-12.414	14.643	10.965	1.00	67.36
ATOM	4539	OH2 TIP	222	10.978	9.734	-1.436	1.00	38.81
ATOM	4540	OH2 TIP	223	11.293	12.362	-1.306	1.00	52.56
ATOM	4541	OH2 TIP	224	34.011	13.162	-1.255	1.00	52.58
ATOM	4542	OH2 TIP	225	31.195	17.923	8.021	1.00	75.88
ATOM	4543	OH2 TIP	226	36.957	11.949	-1.947	1.00	50.99
ATOM	4544	OH2 TIP	227	35.179	3.114	10.888	1.00	58.55
ATOM	4545	OH2 TIP	228	64.027	13.281	26.577	1.00	51.98
ATOM	4546	OH2 TIP	229	36.514	6.155	15.292	1.00	45.57
ATOM	4547	OH2 TIP	230	90.627	4.339	6.386	1.00	56.65
ATOM	4548	OH2 TIP	231	49.907	-11.937	10.792	1.00	53.49
ATOM	4549	OH2 TIP	232	60.296	-10.212	16.610	1.00	79.85
ATOM	4550	OH2 TIP	233	18.154	-21.314	7.018	1.00	53.60
ATOM	4551	OH2 TIP	234	66.186	-1.068	30.882	1.00	56.92
ATOM	4552	OH2 TIP	235	75.153	18.983	20.700	1.00	34.22
ATOM	4553	OH2 TIP	236	-2.885	10.207	3.295	1.00	68.34
ATOM	4554	OH2 TIP	237	5.834	-3.507	25.370	1.00	34.75
ATOM	4555	OH2 TIP	238	35.910	6.163	12.569	1.00	37.31
ATOM	4556	OH2 TIP	239	-5.494	16.637	14.033	1.00	65.17
ATOM	4557	OH2 TIP	240	46.332	-11.698	26.865	1.00	55.30
ATOM	4558	OH2 TIP	241	6.179	6.434	13.895	1.00	45.92
ATOM	4559	OH2 TIP	242	-3.869	-4.958	20.821	1.00	41.96
ATOM	4560	OH2 TIP	243	1.690	-3.598	-0.200	1.00	41.42
ATOM	4561	OH2 TIP	244	86.181	11.454	23.000	1.00	56.22
ATOM	4562	OH2 TIP	245	10.501	7.621	5.627	1.00	77.40
ATOM	4563	OH2 TIP	246	5.007	8.485	2.181	1.00	89.31
ATOM	4564	OH2 TIP	247	64.552	-8.093	20.595	1.00	45.86
ATOM	4565	OH2 TIP	248	11.243	-17.828	13.332	1.00	65.30
ATOM	4566	OH2 TIP	249	42.226	-6.785	14.857	1.00	81.78
ATOM	4567	OH2 TIP	250	2.875	-4.176	22.032	1.00	53.45
ATOM	4568	OH2 TIP	251	72.048	1.134	-2.037	1.00	38.85
ATOM	4569	OH2 TIP	252	50.357	-3.142	32.887	1.00	67.13
ATOM	4570	OH2 TIP	254	57.772	9.500	11.808	1.00	40.03

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ATOM	4571	OH2	TIP	255	43.306	20.459	30.366	1.00	47.59
ATOM	4572	OH2	TIP	256	67.064	16.514	15.765	1.00	57.51
ATOM	4573	OH2	TIP	257	87.612	21.648	5.147	1.00	70.52
ATOM	4574	OH2	TIP	258	21.095	9.853	-9.308	1.00	78.97
ATOM	4575	OH2	TIP	261	71.914	28.544	7.912	1.00	83.90
ATOM	4576	OH2	TIP	262	25.727	-8.133	27.190	1.00	54.87
ATOM	4577	OH2	TIP	263	-18.738	10.877	12.767	1.00	71.80
ATOM	4578	OH2	TIP	264	30.524	11.543	16.329	1.00	46.98
ATOM	4579	OH2	TIP	265	22.211	-16.242	-2.763	1.00	55.17
ATOM	4580	OH2	TIP	266	29.755	9.037	18.396	1.00	67.93
ATOM	4581	C1	MON	1000	67.458	4.500	11.935	1.00	0.00
ATOM	4582	C2	MON	1000	67.015	3.958	10.687	1.00	0.00
ATOM	4583	N3	MON	1000	67.367	2.732	10.160	1.00	0.00
ATOM	4584	C4	MON	1000	66.127	4.618	9.793	1.00	0.00
ATOM	4585	C5	MON	1000	65.620	5.919	10.125	1.00	0.00
ATOM	4586	C6	MON	1000	66.041	6.508	11.380	1.00	0.00
ATOM	4587	C7	MON	1000	66.948	5.809	12.276	1.00	0.00
ATOM	4588	C8	MON	1000	65.933	3.759	8.668	1.00	0.00
ATOM	4589	C10	MON	1000	66.745	2.518	8.922	1.00	0.00
ATOM	4590	C11	MON	1000	65.043	4.051	7.483	1.00	0.00
ATOM	4591	O12	MON	1000	66.862	1.516	8.241	1.00	0.00
ATOM	4592	C13	MON	1000	64.479	2.990	6.570	1.00	0.00
ATOM	4593	C14	MON	1000	63.459	3.330	5.617	1.00	0.00
ATOM	4594	C15	MON	1000	62.923	2.333	4.727	1.00	0.00
ATOM	4595	C16	MON	1000	63.379	0.956	4.754	1.00	0.00
ATOM	4596	C17	MON	1000	64.960	1.637	6.605	1.00	0.00
ATOM	4597	C18	MON	1000	64.418	0.642	5.713	1.00	0.00
ATOM	4598	N19	MON	1000	62.848	-0.025	3.880	1.00	0.00
ATOM	4599	C20	MON	1000	63.429	-1.407	3.816	1.00	0.00
ATOM	4600	C21	MON	1000	61.888	0.343	2.786	1.00	0.00
ATOM	4601	C22	MON	1000	61.085	-0.818	2.152	1.00	0.00
ATOM	4602	N23	MON	1000	61.868	-2.035	1.930	1.00	0.00
ATOM	4603	C24	MON	1000	62.562	-2.492	3.133	1.00	0.00
ATOM	4604	O25	MON	1000	61.481	-2.328	-0.389	1.00	0.00
ATOM	4605	C26	MON	1000	62.001	-2.670	0.659	1.00	0.00
ATOM	4606	C1	MON	1001	5.458	3.340	18.422	1.00	0.00
ATOM	4607	C2	MON	1001	6.049	3.475	19.718	1.00	0.00
ATOM	4608	N3	MON	1001	5.935	2.580	20.763	1.00	0.00
ATOM	4609	C4	MON	1001	6.857	4.573	20.124	1.00	0.00
ATOM	4610	C5	MON	1001	7.121	5.641	19.202	1.00	0.00
ATOM	4611	C6	MON	1001	6.543	5.548	17.877	1.00	0.00
ATOM	4612	C7	MON	1001	5.722	4.412	17.489	1.00	0.00
ATOM	4613	C8	MON	1001	7.250	4.340	21.477	1.00	0.00
ATOM	4614	C10	MON	1001	6.647	3.023	21.886	1.00	0.00
ATOM	4615	C11	MON	1001	8.138	5.242	22.302	1.00	0.00
ATOM	4616	O12	MON	1001	6.735	2.426	22.943	1.00	0.00
ATOM	4617	C13	MON	1001	8.918	4.783	23.509	1.00	0.00
ATOM	4618	C14	MON	1001	9.913	5.641	24.091	1.00	0.00
ATOM	4619	C15	MON	1001	10.654	5.224	25.253	1.00	0.00
ATOM	4620	C16	MON	1001	10.435	3.935	25.881	1.00	0.00
ATOM	4621	C17	MON	1001	8.670	3.508	24.123	1.00	0.00
ATOM	4622	C18	MON	1001	9.416	3.095	25.285	1.00	0.00

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ATOM	4623	N19	MON	1001	11.168	3.525	27.023	1.00	0.00
ATOM	4624	C20	MON	1001	10.831	2.255	27.749	1.00	0.00
ATOM	4625	C21	MON	1001	12.107	4.463	27.725	1.00	0.00
ATOM	4626	C22	MON	1001	13.125	3.821	28.698	1.00	0.00
ATOM	4627	N23	MON	1001	12.570	2.742	29.518	1.00	0.00
ATOM	4628	C24	MON	1001	11.902	1.711	28.725	1.00	0.00
ATOM	4629	O25	MON	1001	13.118	3.569	31.669	1.00	0.00
ATOM	4630	C26	MON	1001	12.610	2.731	30.944	1.00	0.00

SSSD/55034. V01

CLAIMS

What is claimed is:

5

1. A crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

10

2. The crystalline form of claim 1, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

15

3. The crystalline form of claim 2, wherein said receptor protein tyrosine kinase is selected from the group consisting of PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

20

4. The crystalline form of claim 1, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

25

5. The crystalline form of claim 4, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

30

6. The crystalline form of claim 1, comprising one or more heavy metal atoms.

7. The crystalline form of claim 1, wherein said

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protein tyrosine kinase is FGFR.

8. The crystalline form of claim 7, wherein said FGFR is FGFR1.

5

9. The crystalline form of claim 8, defined by atomic structural coordinates set forth in Table 1.

10. The crystalline form of claim 7, comprising at least one compound.

10

11. The crystalline form of claim 10, wherein said compound is a nucleotide analog.

15

12. The crystalline form of claim 11, wherein said nucleotide analog is AMP-PCP.

13. The crystalline form of claim 12, defined by atomic structural coordinates set forth in Table 2.

20

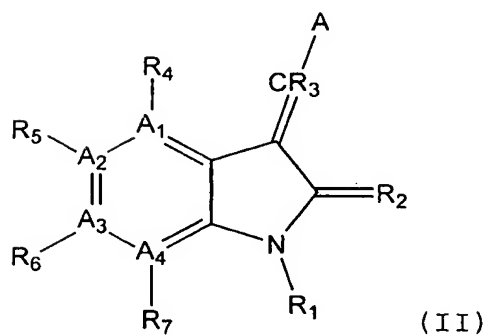
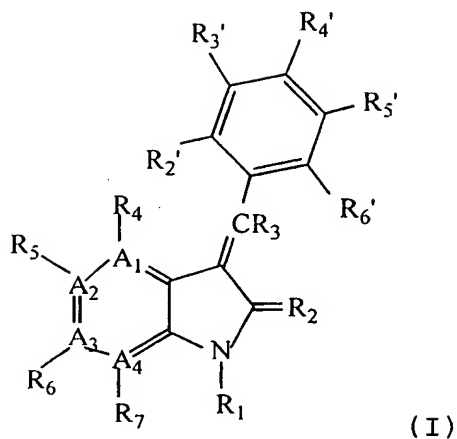
14. The crystalline form of claim 10, wherein said compound is an indolinone compound.

15. The crystalline form of claim 14, wherein said indolinone compound has a structure set forth in formula I or II:

25



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or a pharmaceutically acceptable salt, isomer,  
metabolite, ester, amide, or prodrug thereof, wherein

5 (a) A<sub>1</sub>, A<sub>2</sub>, A<sub>3</sub>, and A<sub>4</sub> are independently carbon or  
nitrogen;

(b) R<sub>1</sub> is hydrogen or alkyl;

(c) R<sub>2</sub> is oxygen in the case of an oxindolinone or  
sulfur in the case of a thiolindolinone;

10 (d) R<sub>3</sub> is hydrogen;

(e) R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> are optionally present and are

either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR' or (ii) any two adjacent R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

(f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR';

(g) n is 0, 1, 2, or 3;

(h) R is hydrogen, alkyl or aryl;

(i) R' is hydrogen, alkyl or aryl; and

(j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R or CONRR'.

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16. The crystalline form of claim 15, wherein said indolinone compound is 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone.

5 17. The crystalline form of claim 15, wherein said indolinone compound is 3-[4-(4-formylpiperazine-1-yl)benzylidenyl]-2-indolinone.

10 18. The crystalline form of claim 16, defined by the atomic structural coordinates of Table 3.

19. The crystalline form of claim 17, defined by the atomic structural coordinates of Table 4.

15 20. The crystalline form of claim 1, having monoclinic unit cells.

20 21. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about  $a=208.3$  Å,  $b=57.8$  Å,  $c=65.5$  Å and  $\beta=107.2^\circ$ .

22. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about  $a=211.6$  Å,  $b=51.3$  Å,  $c=66.1$  Å and  $\beta=107.7^\circ$ .

25 23. The crystalline form of claim 10, comprising one or more heavy metal atoms.

30 24. A polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first

glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal boundary of the catalytic domain.

5

25. The polypeptide of claim 24, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

10

26. The polypeptide of claim 24, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

15

27. The polypeptide of claim 25, wherein said receptor tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

20

28. The polypeptide of claim 26, wherein said non-receptor kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

25

29. The polypeptide of claim 24 having the amino acid sequence shown in SEQ ID NO:4.

30. A method of using the polypeptide of claim 24 to form a crystal, comprising the steps of:

(a) mixing a volume of polypeptide solution with a reservoir solution; and

30

(b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container,

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under conditions suitable for crystallization.

31. A method of obtaining an FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of:

(a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, wherein said polypeptide solution comprises 1 mg/mL to 60 mg/mL FGF-type tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and wherein said reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and

(b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25° °C until crystals form.

32. The method of claim 31, wherein said polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

33. The method of claim 31, wherein said

polypeptide solution comprises a compound.

5 34. A cDNA encoding an FGF receptor tyrosine kinase domain protein, wherein a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.

10 35. A method of determining three dimensional structures of protein tyrosine kinases with unknown structure comprising the step of applying structural atomic coordinates set forth in Table 1, Table 2, Table 3, or Table 4.

36. The method of claim 35, comprising the following steps:

15 (a) aligning a first computer representation of an amino acid sequence of a protein tyrosine kinase of unknown structure with a second computer representation of a protein tyrosine kinase of known structure by matching homologous regions of amino acid sequences of said first computer representation and said  
20 second computer representation;

25 (b) transferring computer representations of amino acid structures in said protein tyrosine kinase of known structure to computer representations of corresponding amino acid structures in said protein tyrosine kinase with unknown structure; and

(c) determining a low energy conformation of the protein tyrosine kinase structure resulting from step (b).

30 37. The method of claim 35, comprising the

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following steps:

(a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals; and

5 (b) determining a low energy conformation of the resulting protein tyrosine kinase structure.

38. The method of claim 35, comprising the following steps:

10 (a) determining the secondary structure of a protein tyrosine kinase structure using NMR data; and

(b) simplifying the assignment of through-space interactions of amino acids.

15 39. The method of any one of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a receptor protein tyrosine kinase.

20 40. The method of claim 39, wherein said receptor protein tyrosine kinase with or without known structure is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

25 41. The method of anyone of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a non-receptor protein tyrosine kinase.

30 42. The method of claim 41, wherein said protein tyrosine kinase with or without known structure is

selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

5           43. A method of identifying a potential modulator  
of protein tyrosine kinase function by docking a  
computer representation of a structure of a compound  
with a computer representation of a structure of a  
cavity formed by the active-site of a protein tyrosine  
10 kinase, wherein said structure of said protein tyrosine  
kinase is defined by atomic structural coordinates set  
forth in Table 1, Table 2, Table 3, or Table 4.

          44. The method of claim 43, comprising the  
following steps:

15           (a) removing a computer representation of a  
compound complexed with a protein tyrosine kinase and  
docking a computer representation of a compound from a  
computer data base with a computer representation of the  
active-site of the protein tyrosine kinase;

20           (b) determining a conformation of the complex  
resulting from step (a) with a favorable geometric fit  
and favorable complementary interactions; and

          (c) identifying compounds that best fit said  
active-site as potential modulators of protein tyrosine  
25 kinase function.

          45. The method of claim 43, comprising the  
following steps:

30           (a) modifying a computer representation of  
compound complexed with a protein tyrosine kinase by the  
deletion of a chemical group or groups or by the



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addition of a chemical group or groups;

(b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and

5 (c) identifying compounds that best fit the protein tyrosine kinase active-site as potential modulators of protein tyrosine kinase function.

10 46. The method of claim 43, wherein said method comprises the following steps:

(a) removing a computer representation of a compound complexed with a protein tyrosine kinase; and

15 (b) searching a data base for data base compounds similar to said compounds using a compound searching computer program or replacing portions of said compound with similar chemical structures from a data base using a compound construction computer program.

20 47. The method of any one of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

25 48. The method of claim 47, wherein said receptor protein tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

30 49. The method of anyone of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

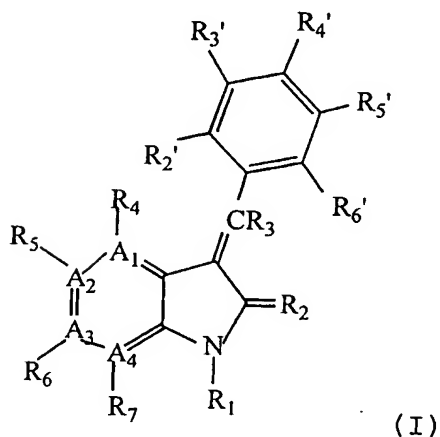
50. The method of claim 49, wherein said protein tyrosine kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

5 51. a potential modulator of protein tyrosine kinase function identified by the method of any one of claims 43, 44, 45, or 46.

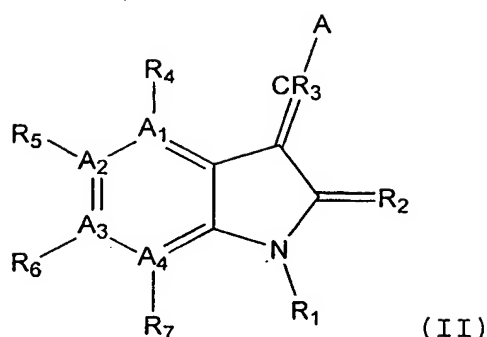
10 52. The potential modulator of claim 51, wherein said modulator is selected from a computer data base.

53. The potential modulator of claim 51, wherein said modulator is constructed from chemical groups selected from a computer data base.

15 54. The potential modulator of protein tyrosine kinase function of claim 51, wherein said modulator is an indolinone compound of formula I or II:



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or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

(a) A<sub>1</sub>, A<sub>2</sub>, A<sub>3</sub>, and A<sub>4</sub> are independently carbon or nitrogen;

(b) R<sub>1</sub> is hydrogen or alkyl;

(c) R<sub>2</sub> is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;

(d) R<sub>3</sub> is hydrogen;

(e) R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> are optionally present and are either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR' or (ii) any two adjacent R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

(f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R,

SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR';

(g) n is 0, 1, 2, or 3;

(h) R is hydrogen, alkyl or aryl;

(i) R' is hydrogen, alkyl or aryl; and

(j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R or CONRR'.

55. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, comprising the following steps:

(a) administering said potential modulator to cells;

(b) comparing the level of protein tyrosine kinase phosphorylation between cells not administered the potential modulator and cells administered said potential modulator; and

(c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on

the difference in the level of protein tyrosine kinase phosphorylation.

56. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, wherein said method comprises the following steps:

(a) administering a preparation of said potential modulator to cells;

(b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and

(c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on the difference in the rate of cell growth.

57. A method of treating a disease associated with a protein tyrosine kinase with inappropriate activity in a cellular organism, wherein said method comprises the steps of:

(a) administering a modulator of protein tyrosine kinase function to the organism, wherein said modulator is in an acceptable pharmaceutical preparation; and

(b) activating or inhibiting the protein tyrosine kinase function to treat the disease.

58. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

59. The method of claim 58, wherein said receptor protein tyrosine kinase is selected from the group containing FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

5

60. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

10

61. The method of claim 60, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

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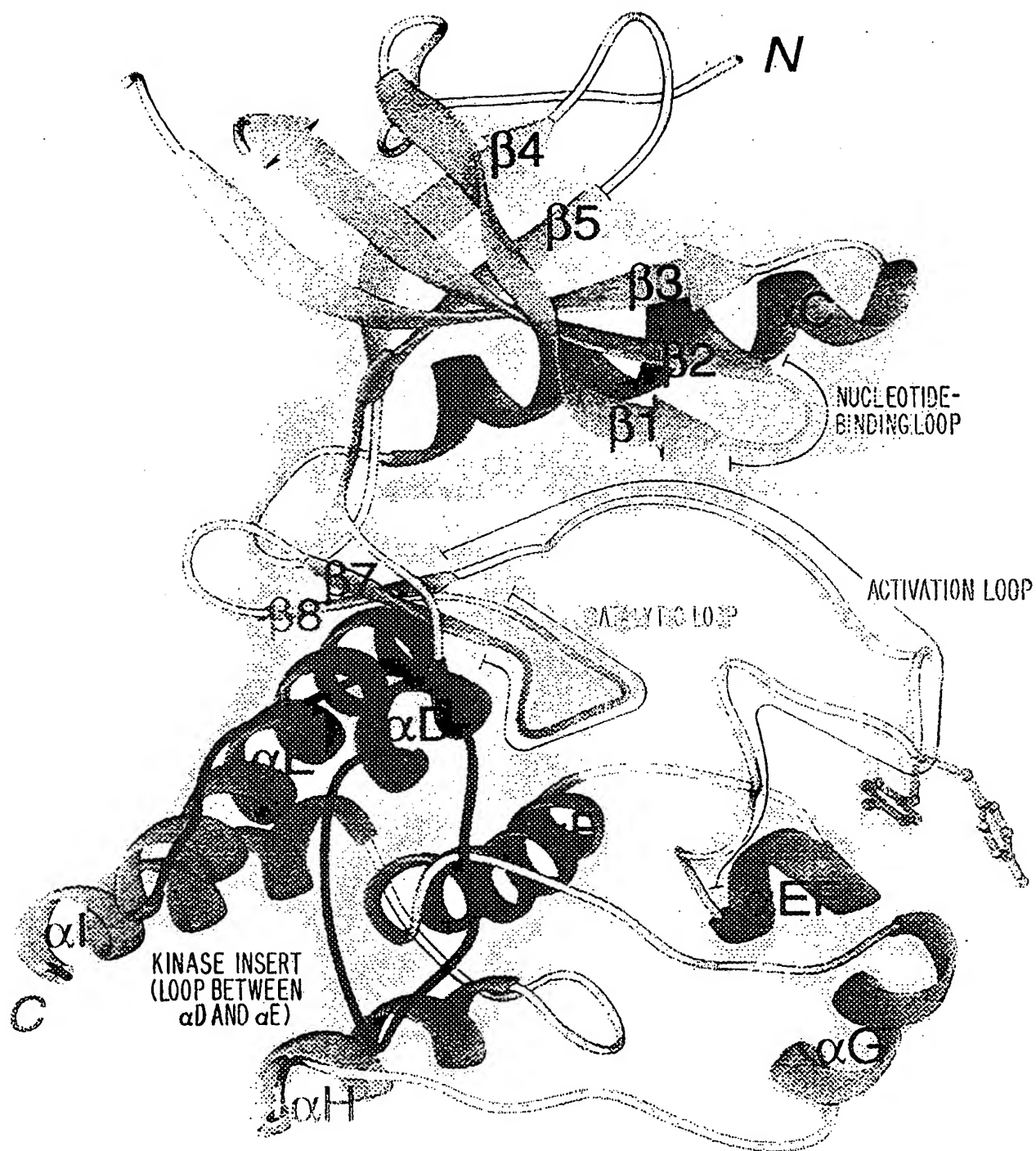


FIG. 1.

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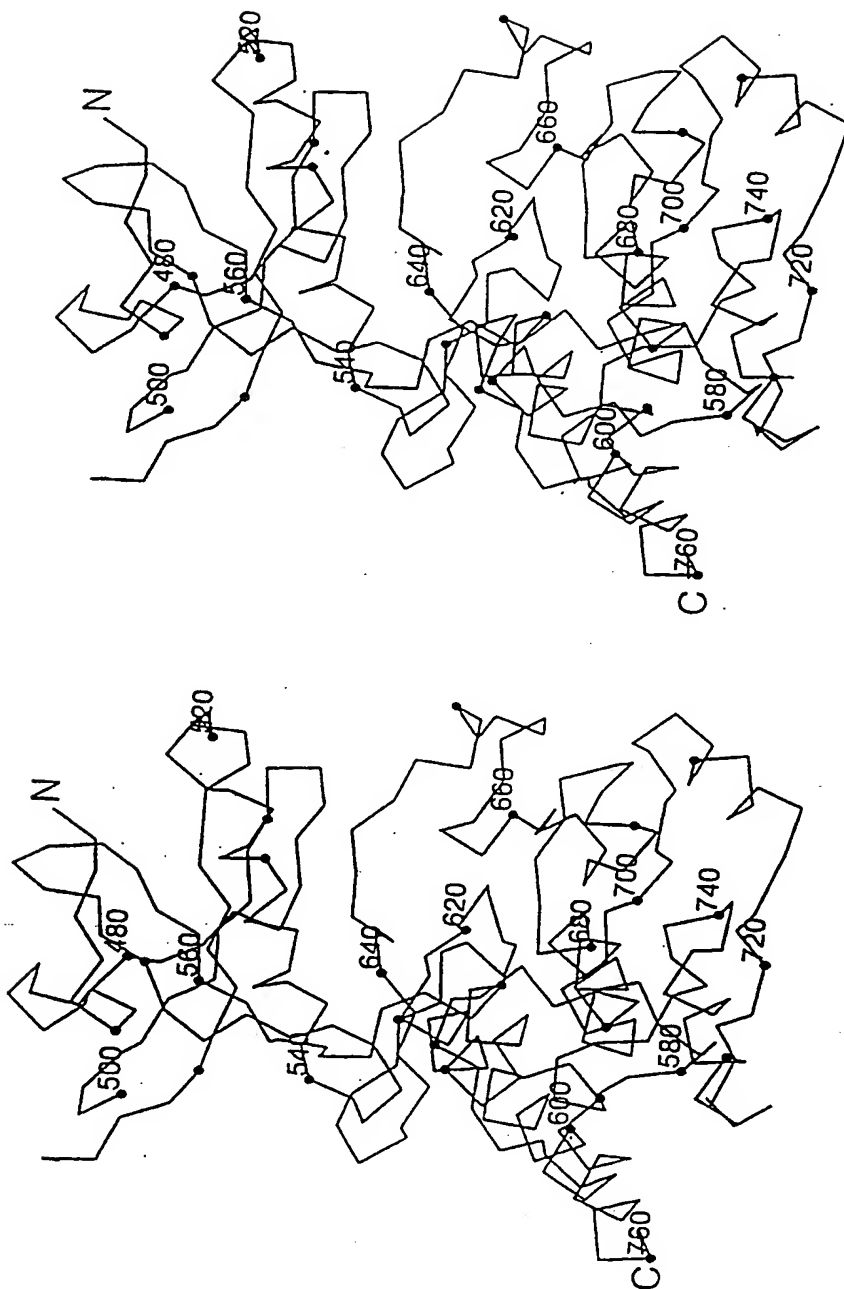


FIGURE 2



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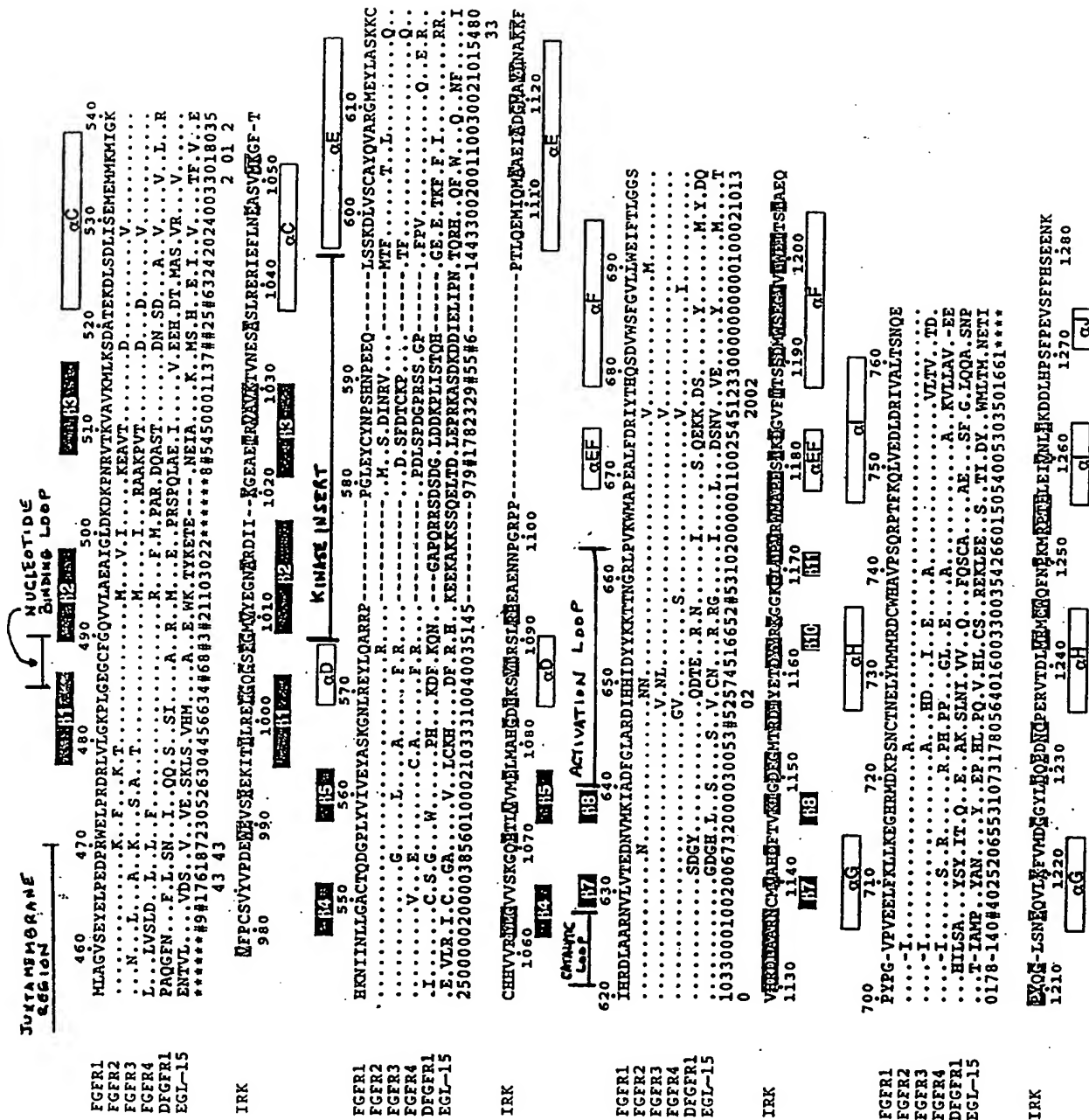


FIG. 4A.

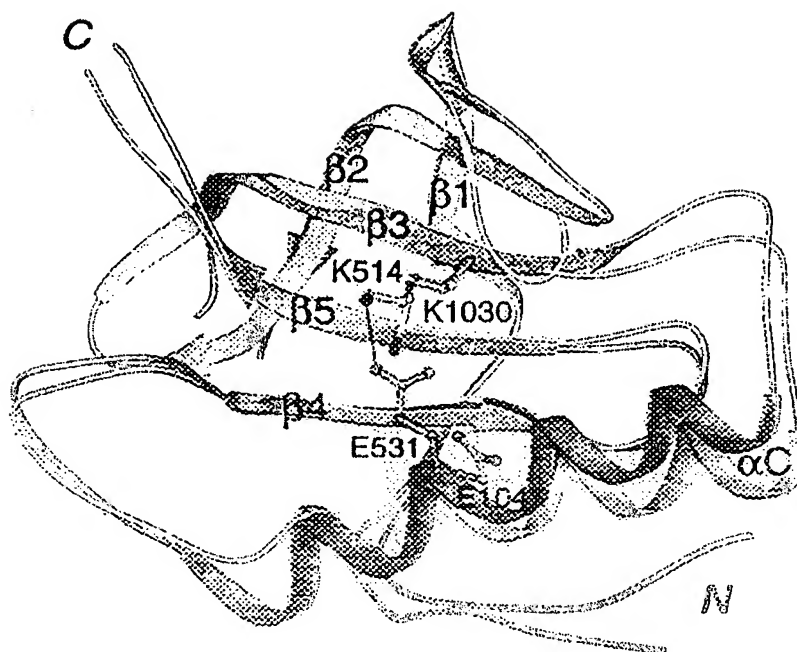
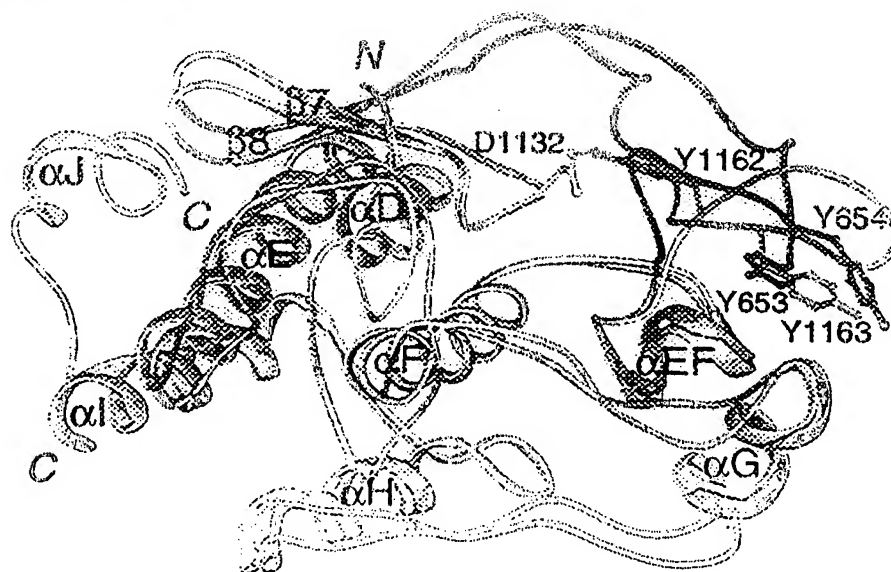
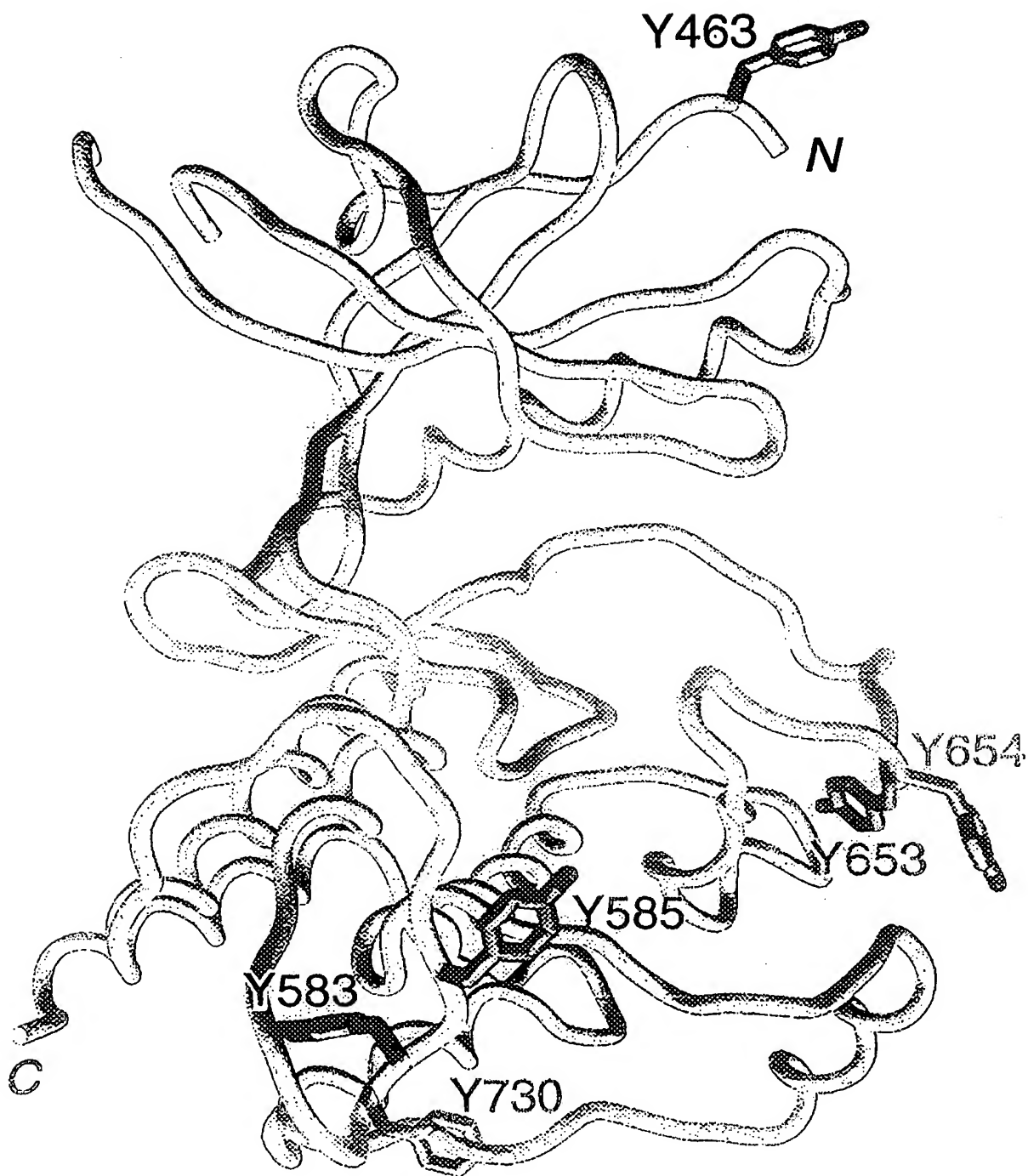


FIG. 4B.



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*FIG. 5.*

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## GLYCINE

RICH

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FGFR1_h	LP-ED-PRW-	E--LPRDRLV	LGKPIGEGCF	QOVLAEAIG	LDK-DK----	-----PNRV	TKVAVKMLKS	-DATEKDLS	LISEMEMMKM
EGFR_h	PNQALLRILK	ETEFKKIKV-	----LQSGAF	GTVYKGLWIP	E-G-EK----	-----V-K	IPVAKELRE	-ATSPKANKE	ILDEAYVMAS
INSR_h	VYVPDE--W-	E--VSREKIT	LLRELQGSF	GAUYEGNARD	IIK-GE----	-----A-E	TRVAVKTVNE	-SASLRERIE	FLNEASVMKG
PDGFra_h	LP-YD-SRW-	E--FPRDGLV	LGRVLGSGAF	GKVVEGTAYG	LSR-SQ----	-----P-V	MKVAVKMLKP	-TARSSEKQA	LMSELKIMTH
KDR_h	-P-YDASKW-	E--FPRDRLN	LGKPIGSGAF	GQIEEADAFG	IDK-TA----	-----T-C	RTVAVKMLKE	-GATHSEHRA	LMSELKILIH
CCK4_h	HSTSD--KM-	H--FPRSSLQ	PITTLGKSEF	GEVFLAKAQG	LEE-GV----	-----A-E	TLVLVKSQ-	-SKDEQQQLD	FRRELEMFCK
MET_h	AVQHVVGPS	SLI-----VH	FNEVIGRGHF	GCVYHGTLLD	N-D-GK----	-----K	IHCAVKSILNR	-ITDIGEVSQ	FLTEGIIMKD
TRKA_h	FSDACVHHIK	-----RRDIV	LKWEILGEGAF	GKVFLAECHN	LLP-EQ----	-----D-K	MLVAVKALK-	-EASESARQD	FORAEALLTM
AXL_h	--KEKL--R-	DVMVDRHKVA	LGKTLGEGEF	GAVMEGQLNQ	D-D-SI----	-----	LKVAVKIMKI	AICTRSELED	FLSEAVCMKE
TIE_h	-P-EPL--S-	YPVLEWEDIT	FEDLIGEGNF	GQVIRAMIKK	D-GLK-----	-----	MNAATKMLKE	-YASENDHRD	FAGELEVLCK
EPH_h	WSNFPS--R-	E--LDPAWLM	VDTVIGEGEF	GEVYRGTLRL	P-S-QD----	-----C	KTVAIKTLKD	-TSPGGQWVN	FLREATIMQ
RYK_h	--KGKV--K-	DIAISRERIT	LKDVLQEGTF	GRIFHGILID	EKD-PN----	-----K-E	KQAFVKTVD	-QASEIQVTM	MLTESCKLRG
DDR_h	GDG-P-PRV-	D--FPRSRLR	FKEKLGEGQF	GEVHLCCEVDS	PQD-LVSLDF	PLNVRKGH-P	LLVAVKILRP	-DATKNARN	FLKEVKIMSR
ROS_h	E--EIE--N-	LPAPPREKLT	LRLILGSGAF	GEVYEGTAVD	ILGVS-----	-----G-E	IKVAVKTLKK	-GSTDQEKIE	FLKEAHLMSK
RET_h	IL-ED-PKW-	E--FPRKNLV	LGKTLGEGEF	GKVVKATAFH	LKG-RA----	-----G-Y	TTVAVKMLKE	-NASPSELRD	LLSEFNVLKQ
LTK_h	-P-LP-PGVT	E--VSPANVT	LLRALGEGAF	GEVYEGLVIG	LPG-DS----	-----S-P	LQVAKTLPE	-LCSPQDELD	FLMEALIISK
ROR1_h	KPKSKA--K-	E--LPLSAVR	FMEELGEGAF	GKIYKGHLYL	P-G-MD----	-----H-A	QLVAKTLKD	-YNNPQOWME	FQOEASLMAE
MUSK_m	NPKLLS--L-	E--YPRNNIE	YVRDIGEGAF	GRVFQARAPG	LLP-YE----	-----P-F	TMVAVKMLKE	-EASADMQAD	FORAEALMAE

III

II

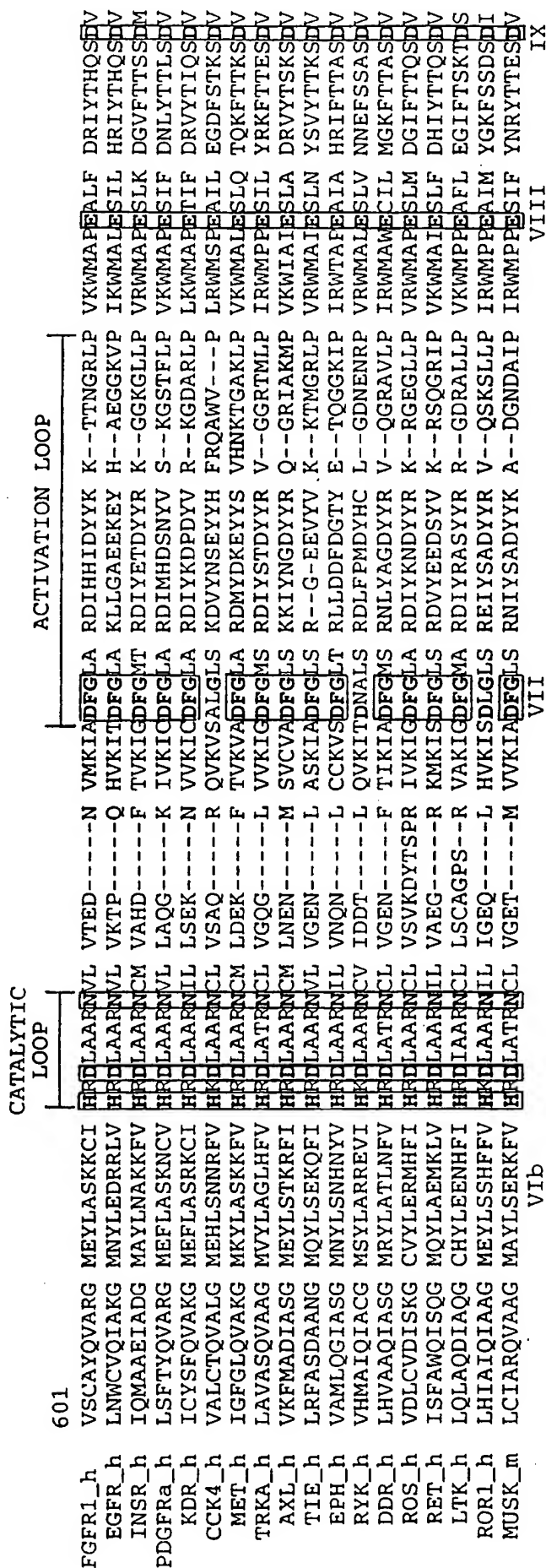
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Fig. 6A-1

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KINASE INSERT											Via
538	IGKHKNIINL	LGACTQD-GP	L-----YVIV	EYASKGNLRE	YLQ-ARRPPG	LEYCYNPSH-	-----	NP----	E-	-EQL-SSKDL	
FGFR1_h	VDN-PHVCRL	LGICLTS-TV	Q-----LI-T	QLMPFGCLLD	YVR-EHK-DN	-----	-----	-----	-----	---IGSQY-L	
EGFR_h	FTC-HHVVRL	LGVSCKG-QP	T-----LVVM	ELMAHGDLS	YLR-SLRP--	-----	ENN-----	PG-----	R-	-PPP-TLQEM	
INSR_h	LGPHLNIVNL	LGACTKS-GP	I-----YIIT	EYCFYGDVLN	YLR-KNR-DS	F---L--SH-	-----	-----	HPE(87)	SEGL-TLLDL	
PDGFra_h	IGHHLNVVNL	LGACTKPGGP	L-----MVIV	EYCFYGNLST	YLR-SKR-NE	F---V--PY-	-----	-----	---KTK(55)	KDFL-TLEHL	
KDR_h	LNH-ANVVRL	LGCREA-EP	H-----YMLV	EYVDLGDLLQ	FLRISKSKDE	K---L-----	-----	-----	---K---	-QPL-STKQK	
CCK4_h	FSH-PNVLSL	LGICLRS-EG	-----SPLVVL	PYMKHGDLRN	FIR-NE----	-----	HN-----	-----	-----	---P-TVKDL	
MET_h	LQH-QHIVRF	FGVCTEG-RP	L-----LMVF	EYMRHGDLNR	FLR-SHGPPA	K---LLAGGE	DVA-----	-----	P-	-GPL-GLGQL	
TRKA_h	FDH-PNVMRL	IGVCFQGSER	ESFPAPVVIL	PFMKHGDLS	FLLYSRLGD-	-----	-----	-----	Q---	-VYL-PTQML	
AXL_h	LGHPNIINL	LGACKNR-GY	L-----YIAI	EYAPYGNLLD	FLR-KSRVLE	TDPAFAREH-	-----	GT-----	A-	-STL-SSRQL	
TIE_h	FSH-PHILHL	EGVTKR-KP	I-----MIIT	EFMENGALDA	FLR-ERE-DQ	-----	-----	-----	-----	---L-VPGQL	
EPH_h	LHH-RNLLPI	THVCIEE-GE	-----KPMVIL	PYMWGNLKL	FLRQ-----	CKL--VEA NN	-----	-----	P-	-QAI-SQODL	
RYK_h	LKD-PNIIRL	LGVCVQD-DP	L-----CMIT	DYMENGDLNQ	FLS-AHQLED	KA-----	EGA-----	PGDQAAQG-	PTI-SQDML		
DDR_h	FNH-PNLIKQ	LGVCCLN-EP	Q-----YIIL	ELMEGDDLTT	YLR-KARM-A	-----	-----	TFY--G-	PLL-TLVDL		
ROS_h	VNH-PHVIKL	YGACSDQ-GP	L-----LLIV	EYAKYGSRLG	FLR-ESRKVG	PYLGSGGSR	NSSLDHPDE	RA-----	---	-L-TMGDL	
RET_h	FRH-QNIVRC	VGLSLRA-TP	R-----LILL	ELMSGGDMKS	FLR-HSRP-H	-----	-----	LGQ----	P-	-SPL-VMRDL	
LTK_h	LHH-PNIVCL	LGAVTQE-QP	V-----CMLF	EYINQGDLEH	FLI-MRSP-H	SDVGCSSDED	GTVK-----	-----	---	-SSL-DHGDF	
ROR1_h	FDN-PNIVKL	LGCAVAG-KP	M-----CLLF	EYMAVGDLINE	FLR-SMSP-H	TVCSL--SHS	DLSTRARVSS	PG-----	P-	-PPL-SCAEQ	
MUSK_m											

Fig. 6A-2



**Fig. 6A-3**

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684  
 FGFR1\_h WSGV-LLWE IFTLGG-SPY P-GVPVEE--  
 EGFR\_h WSGV-TVWE LMTFGS-KPY D-GIPASE--  
 INSR\_h WSGV-VLWE ITSLAE-QPY Q-GLSNEQ--  
 PDGFRa\_h WSGI-LLWE IFSLGG-TPY P-GMMVDS--  
 KDR\_h WSGV-LLWE IFSLGA-SPY P-GVKIDE--  
 CCK4\_h WAFGV-LMWE VFTHGE-MPH G-GQADDE--  
 MET\_h WSGV-VLWE LMTRGA-PPY P-DVNTFD--  
 TRKA\_h WSGV-VLWE IFTYGG-QPW Y-QLSNTN--  
 AXL\_h WSGV-TMWE IATRGQ-TPY P-GVENSE--  
 TIE\_h WSGV-LLWE IVSLGG-TPY C-GMTCAE--  
 EPH\_h WSGI-VMWE VLSFGD-KPY G-EMSNQE--  
 RYK\_h WAFGVNSLWE LMTLGG-TPY TLDIDPFE--  
 DDR\_h WAFGV-TVWE VMLCRAQPF G-QLTDEQVI  
 ROS\_h WSGI-LIWE ILTLGH-QPY P-AHSNLD--  
 RET\_h WSGV-LLWE IVTLGG-NPY P-GIPPER--  
 LTK\_h WSGV-LLWE IFSLGY-MPY P-GRTNQE--  
 ROR1\_h WSGV-VLWE IFSFGL-QPY Y-GFSNQE--  
 MUSK\_m WAYGV-VLWE IFSYGL-QPY Y-GMAHEE--

763  
 RPTFKQLVED LDRIVALTSN  
 RPKFRELIIE FSKMARDPQR  
 RPTFLEIVNL LKDDLHPSFP  
 RPSFYHLSEI VENLLPGQYK  
 RPTFSELVEH LGNLLQANAQ  
 RPSFSEIASA LGDSTVDSPK  
 RPSFSELVSR ISAIFFSTFIG  
 RSHIKDVHAR LQALAQAPPV  
 RPSFTELRED LENTLKALPP  
 RPPFAQIALQ LGRMLEARKA  
 RPHFQKLQAH LEQLLANPHS  
 RPRFQQLVQC LTFEHAALGA  
 RPPFSQLHRF LAEDALNTV-  
 RPTFHRIONQ LQLFRRNFFLN  
 RPFADISKD LEKMMVKKRRD  
 RPSFASILER LQYCTQDPDV  
 RPRFKDIHVR LRSWEGLSH  
 RPSFCSIHRI LQRMCEAEG

NCTNELYMM RDCWHAVPSQ  
 ICTIDVYMM VKCMIDADS  
 NCPEVTDLM RMCWDFNPKM  
 HATSEVYEIM VKCMNSEPEK  
 YTTPEMYQTM LDCWHGEPSP  
 GCPSKLYRLM QRCWALSPKD  
 YCPDPLYEVM LKCMHPKAEM  
 ACPEVYAIM RGCWOREPQQ  
 DCLDGLYALM SRCWELNPQD  
 NCDDEVYELM RQCWRDRPYE  
 DCPAPLYELM KNCWAYDRAR  
 TCPDELFAVM ACOWALDPPEE  
 ACPOGLYELM LRCWSRESEQ  
 NCDDDLWNLM TQCWAQEPDQ  
 NCSEEMYRLM LQCMKQEPDK  
 GCPGPVYRIM TQCWQHEPEL  
 DCPPRMYSLM TECWNEIPSR  
 NCPLELYNLM RLCWSKLPAD

LF-KLL KEGHRMDKPS  
 IS-SIL EKERLPQPP  
 VL-KFV MDGGYLDQPD  
 TFYNKI KSGYRMKPD  
 EFCRRL KEGTRMRAPD  
 VLADLQ AGKARLPQPE  
 IT-VYL LQGRRLQPE  
 AI-DCI TOGRELERPR  
 IY-DYL RQGNRLKQPA  
 LY-EKL PQGYRMEQPR  
 VM-KSI EDGYRLPPV  
 MAA-YL KDGYRIAQPI  
 ENAGEFFRDQ GRQVLSRPP  
 VL-NYV QTGGRLEPPR  
 LF-NLL KTGHRMERPD  
 VL-DFV VGGGRMDPPR  
 VI-EMV RKRQLPCSE  
 VI-YVY RDGNILACPE

X  
 XI

Fig. 6A-4

465

FGFR1_h	LPEDPRWELP	RDRVLGK-P	IGGCFQVV	LAEAIGLDKD	KPNRVTKVAV	KMLKSDATEK	DLSDLISEME	MMKMI-GKHK
SRC_h	GLAKDAWEIP	RESLRLEV-K	IGQCFGEVW	MGW-----	NGT--TRVAI	KTLKPGTMSP	-E--AFLQ-E	AQVMKKLRHE
BRK_h	LPHWDDWERP	REEFTLCR-K	IGSGYFGEVF	EGLW-----	KDR--VQVAI	KVISRDNLH	-Q--QMLQSE	IQAMKKLRHK
BTK_h	GLGYSWEID	PKDLTFLK-E	IGTQFGVVK	YGKW-----	RGQYD--VAI	KMIKEGSMSE	-D--EFIE-E	AKVMMNLSHE
CSK_h	EFYRSGWALN	MKELKLLQ-T	IGKGEFGDVM	LGDY-----	RGN---KVAV	KCIKNDA-TA	-Q--AFL-AE	ASVMTQLRHS
ABL_h	SPNYDKWEME	RTDITMKH-K	IGGQYGEVY	EGVW-----	K-KYSLTVAV	KTLKEDTMEV	-E--EFLK-E	AAVMKEIKHP
ZAP70_h	LKDKKLF-LK	RDNLLIADIE	IGGNEFGSVR	QGVY---RM	RKKQ-IDVAI	KVLKQG--TE	KADTEEMRE	AQIMHQLDNP
FES_h	AVPKDKWVLN	HEDLVLE-Q	IGRNFCEVF	SGR-----	LRADNTLVAV	KSCRETLPD	LKAK-FLQ-E	ARILKQYSHP
FAK_h	MPSTRDYEIQ	RERIELGRC-	IGGQFGDVH	QGIY---MS	PENPALAVAI	KTCNC--TS	DSVREKFLQ	ALTMROQFDHP
JAK1_h	PTEVDPTHFE	KRFLKRIR-D	IGGCHFGKVE	LCRY---DP	EDNTGEQVAV	KSLKPE--SG	GNHIALDKKE	IEILRNLYHE
ACK_h	PLQSLTCLIG	EKDLRLLE-K	IGGSGFGVVR	RGEW---DA	PSGKTVSVAV	KCLKPDVLSQ	PEAMDDFIRE	VNAMHSLDHR

III

II

I

543

FGFR1_h	NIINLLGACT	-QDGP-LYVI	VEYASKGNLR	EYLQARRPPG	LEYCYNPSHN	PEEQSSKDL	VSCAYQVARG	MEYLASKKCI
SRC_h	KLVLQYAVVS	-E-EP-IYIV	TEYMSKGSLL	DFLKET---	-----	-GKYLRLPQL	VDMAAQIASG	MAYVERMNYV
BRK_h	HILALYAVVS	VG-DP-VYII	TELMAGKSLL	ELLRDS---	-----	-EKVLPVSEL	LDAWQVAEG	MCYLESQNYI
BTK_h	KLVLQYGVCT	KQR-P-IFII	TEYMANGCLL	NYLRE-M---	-----	-RHRFQTQQL	LEMCKDVCEA	MEYLESKQFL
CSK_h	NLVQLLGIVV	EEKGG-LYIV	TEYMAKGSIV	DYLRSG---	-----	-RSVLGGDCL	LKFSLDVCEA	MEYLEGNFV
ABL_h	NLVQLLGVCV	REP-P-FYII	TEFMTYGNLL	DYLREC---	-----	-RQEVNAVVL	LYMATQISSA	MEYLEKKNFI
ZAP70_h	YIVRLIGVCQ	AEA---LMLV	MEMAGGGPLH	KFLVGK---	-----	-REEIPVSNV	AELLHQVSMG	MKYLEEKNFV
FES_h	NIVRLIGVCT	-QKQP-IYIV	MELVQGGDFL	TFLRTE---	-----	-GARLRVKTL	LQMVGDAAAG	MEYLESKCCI
FAK_h	HIVKLIGVIT	ENP---VWII	MELCTLGELR	SFLQVR---	-----	-KYSLDLASL	ILYAYQLSTA	LAYLESKRFB
JAK1_h	NIVKYKGICT	EDGGNGIKLI	MEFLPSGSLK	EYLPKN---	-----	-KNKINLKQQ	LKYAVQICKG	MDYLGSRQYV
ACK_h	NLIRLYGVVL	TPP---MKMV	TELAPLGSL	DRLRKH---	-----	-QGHFLLGTL	SRYAVQVAEG	MGYLESKRFI

V

IV

Via

Vib

Fig. 6B-1



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621	FGFR1_h	HRDLAARNVL	VTEDNVMKIA	DFGLARDIH-	HIDYKKTNN	GRLPVKWMAP	EAL-FDRIYT	HQSDVWSFGV	LLWEIFTLGG
	SRC_h	HRDLRAANIL	VGENLVCKVA	DFGLARLIE-	DNEYTARQGA	-KFPIKWTAP	EALYGR-FT	IKSDVWSFGI	LLTELTTKGR
	BRK_h	HRDLAARNIL	VGENTLCKVG	DFGLARLIK-	EDVYLSDH-H	-NIPYKWTAP	EALSRGH-YS	TKSDVWSFGI	LLHEMFSGQ
	BTK_h	HRDLAARNCL	VNDQGVVKVS	DFGLSRYVL-	DDEYTSSVGS	-KFPVRSPP	EVLMSK-FS	SKSDIWAAGV	LMWEIYSLGK
	CSK_h	HRDLAARNVL	VSEDNVAKVS	DFGLTK----	-EASSTQDTG	-KLVPKWTAP	EALREKK-FS	TKSDVWSFGI	LLWEIYSFGR
	ABL_h	HRDLAARNCL	VGENHLVKVA	DFGLSRLMT-	GDTYTAHAGA	-KFPIKWTAP	ESLAYNK-FS	IKSDVWAAGV	LLWEIATYGM
	ZAP70_h	HRDLAARNVL	LVNRHYAKIS	DFGLSKALGA	DDSYTTARSA	GKWPLKWIAP	ECINFRK-FS	SRSDDVWSYGC	TMWEALSYGQ
	FES_h	HRDLAARNCL	VTEKNVLKIS	DFGMSREEA-	DGVYAAASGGS	RQVPVKWTAP	EALNYGR-YS	SESDVWSFGI	LLWETFSLGA
	FAK_h	HRDLAARNVL	VSSNDCVKLG	DFGLSRYME-	DSTYYKA-SK	GKLPIKWMAP	ESINFRR-FT	SASDDVWMFGV	CMWEILMHGV
	JAK1_h	HRDLAARNVL	VESEHQVKIG	DFGLTKAIET	DKEYYTVKDD	RDSPVFWYAP	ECLMQSK-FY	IASDDVWSFGV	TLHELITYCD
	ACK_h	HRDLAARNLL	LATRDLVKIG	DFGLMRALPQ	NDDHYVMQEH	RKVPFAWCAP	ESLKTRT-FS	HASDDTWMFGV	TLWEMFTYGQ
				VII			VIII		
							IX		
699	FGFR1_h	S-----	-----PYPGVP	VEELFKLLKE	-GHRMDKPSN	CTNELYMMMR	DCMHAVPSQR	PTFKQLVEDL	DRIVALTSNQ
	SRC_h	V-----	-----PYPGMV	NREVLQDQVER	-GYRMPCPPE	CPESLHDLMC	QCMRKEPER	PTFEYLQAF	EDYFTSTEPQ
	BRK_h	V-----	-----PYPGMS	NHEAFLRVDA	-GYRMPCPPE	CPPSVHKLML	TCWCRDPEQR	PCFKALRERL	SSFTSYENPT
	BTK_h	M-----	-----PYERFT	NSETAEHIAQ	-GLRLYRPHL	ASEKVYTIMY	SCWHEKADER	PTFKILLSNI	LDVMEDES--
	CSK_h	V-----	-----PYPRIP	LKDVVPRVEK	-GYKMDAPDG	CPPAVYEVNK	NCWHLDAAMR	PSFLQLREQ	EHIKTHELHL
	ABL_h	S-----	-----PYPGID	LSQVYELLEK	-DYRMERPEG	CPEKVYELMR	ACWQWNPDDR	PSFAEIHQAF	ETMFQESSIS
	ZAP70_h	K-----	-----PYKMK	GPEVMAFIE-	QGKRMCEPPE	CPPELYALMS	DCWIKWEDR	PDFLTVEQRM	RACYYSLSK
	FES_h	S-----	-----PYPNLS	NQQTREFVEK	-GGRLLPCPEL	CPDAVFRIME	QCWAYEPGQR	PSFSTIYQEL	QSIR--KRHR
	FAK_h	K-----	-----PFQGVK	NNDVIGRIE-	NGERLPMPPN	CPPTLYSLMT	KCMAYDPSRR	PRFTELKAQL	STILEEKAQ
	JAK1_h	SDSSPMALFL	KMIGPTHGQM	TVTRLVNTLK	EGKRLPCPPN	CPDEVYQLMR	KCMWFQPSNR	TSFQNLIEGF	-----EALLK
	ACK_h	E-----	-----PWIGLN	GSQILHKIDK	EGERLPRPED	CPQDIYNVMV	QCWAHKPEDR	PTFVALRDFL	LEAQPTDMRA
				X			XI		

Fig. 6B-2



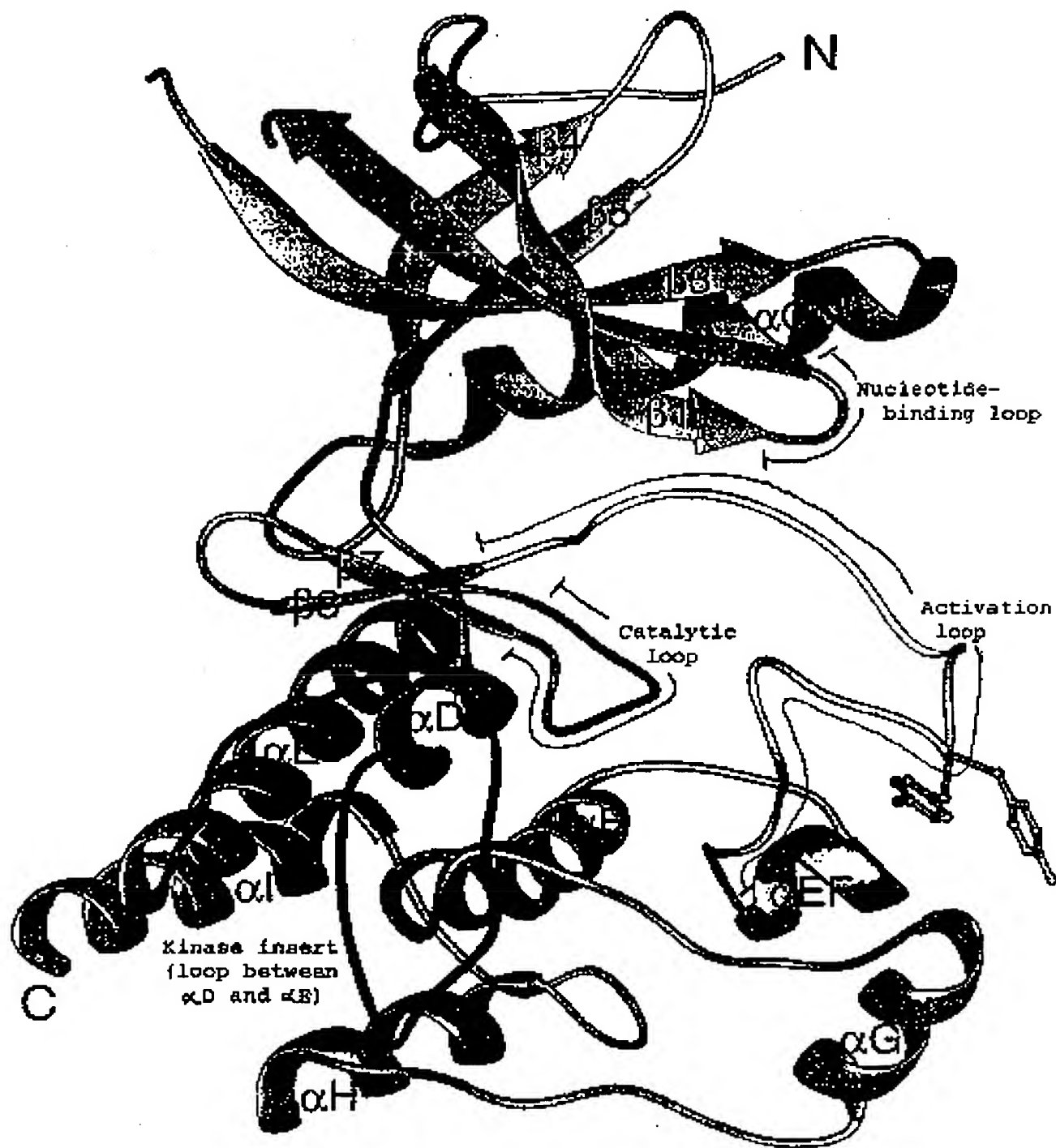


FIGURE 1

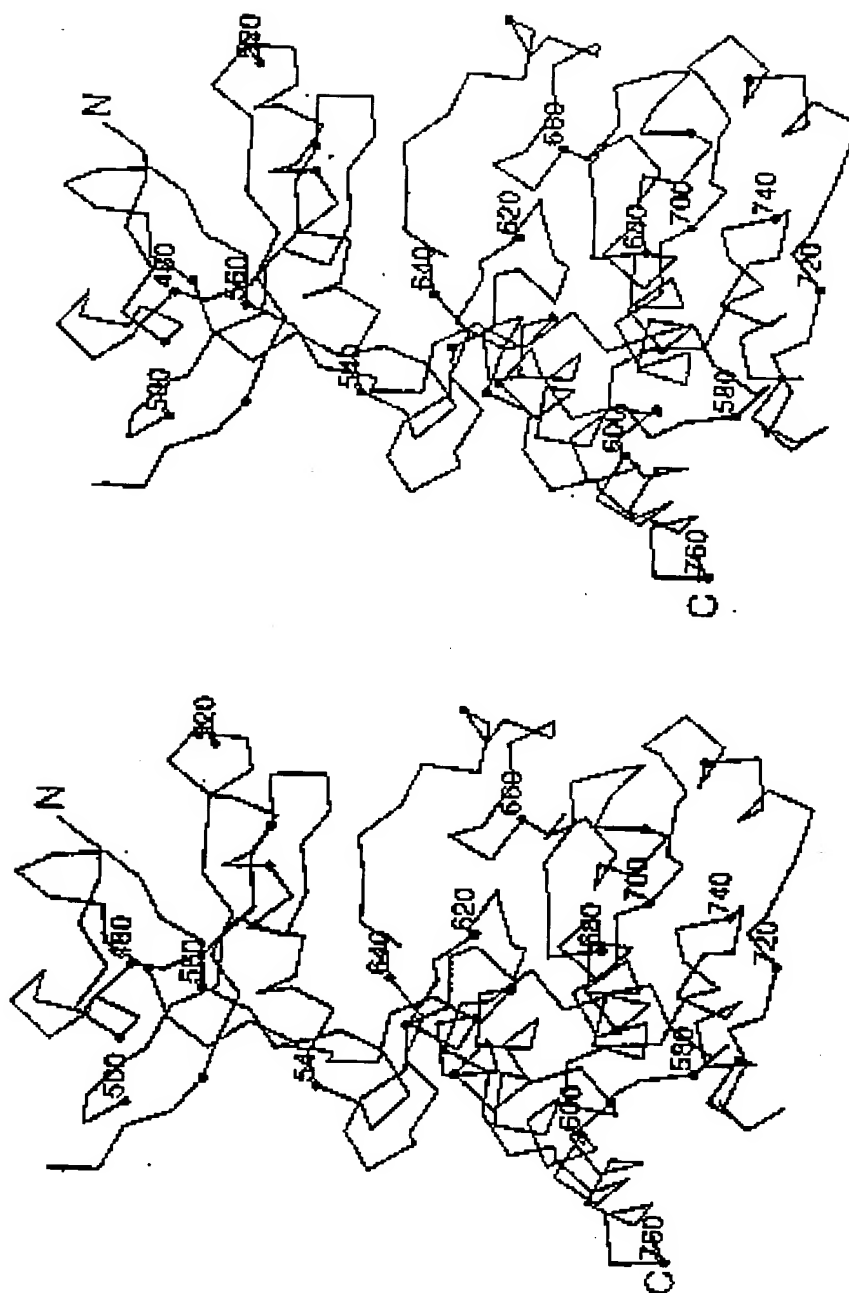


FIGURE 2



FIGURE 4A

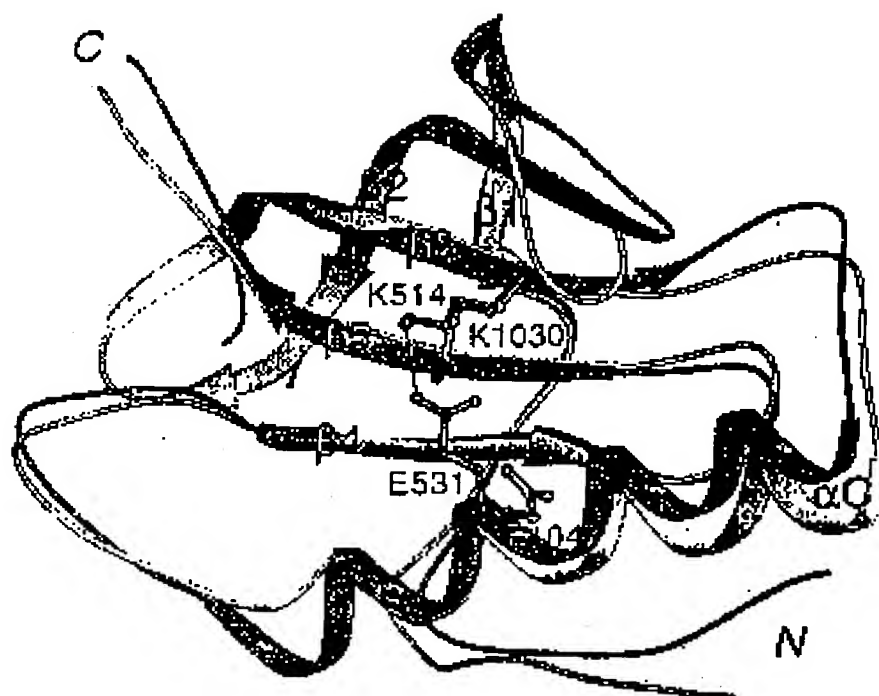
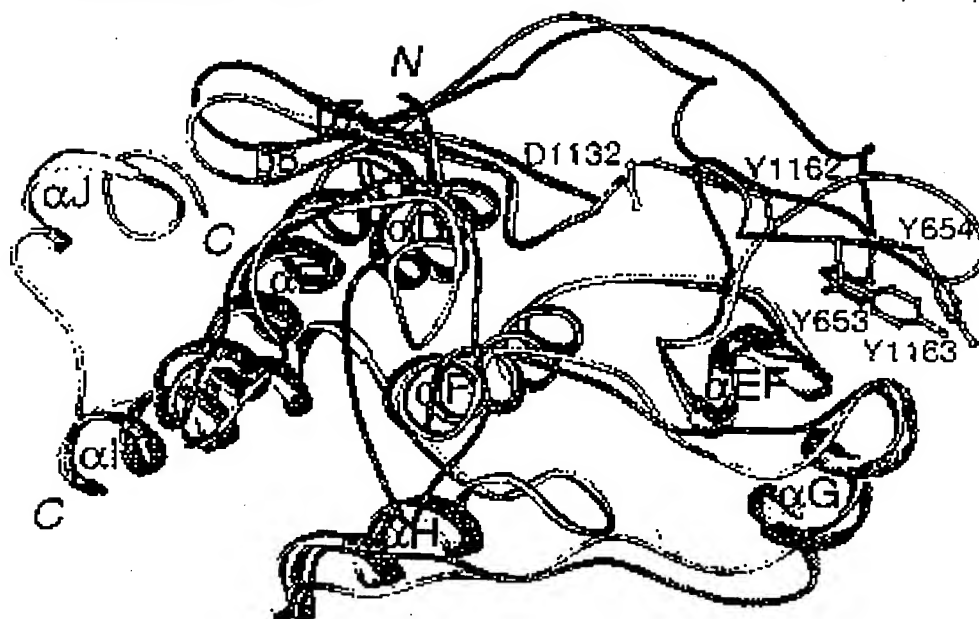


FIGURE 4B



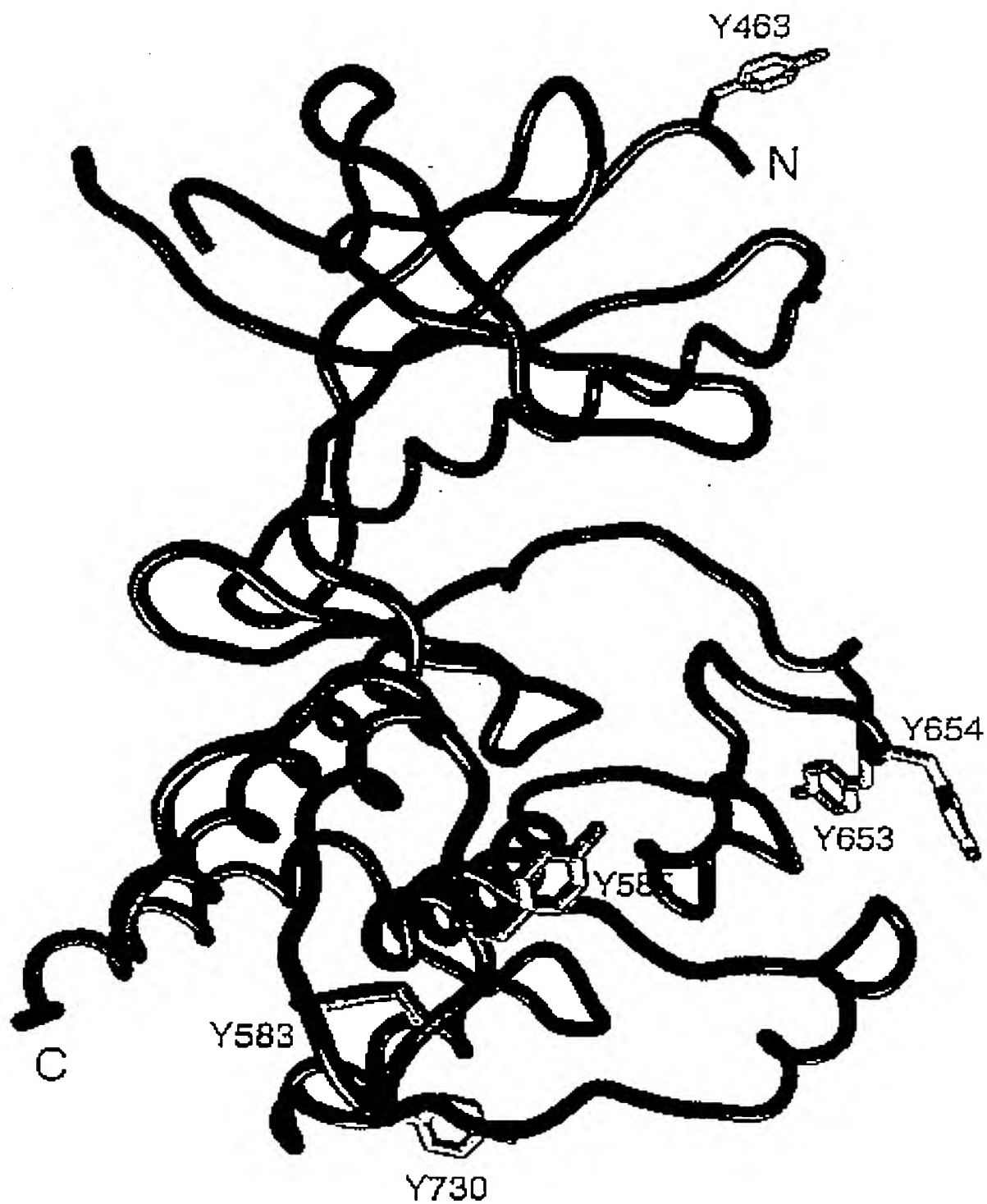


FIGURE 5

GLUCOSE  
RICH

466	FFPR1_h	LP-ED-PRV	E--CPORLY	CONPLET	COVLAETIC	LDC-DK---	-----PWRV	TCVAMTLES	-OATERKASO	4158HNNKKA
	EGFR_h	PHOALLAILK	STEFKKEV	-----LADCF	ETVYECVLP	E-G-EE---	-----Y-K	IPVAMHLSR	-STIPRAHKE	ILDRATVMA3
	INSR_h	VYVPOE--V	E--YSEKIT	CLNULCEBF	EMVYEGHARD	IKK-DE---	-----A-E	TRVAVTYNE	-SALPAGKIE	PLNEASYMAG
	POBPR_h	LP-TO-SRV	E--PPROLY	LGAVLECAF	CKVVESTAYE	LGR-SO---	-----P-V	HCYAVHLLCP	-YASBEEKSA	CHMLKIMTK
	KDR_h	-P-YDASKV	E--PPRDMH	LGKPLCEAF	CKSTEADAPR	IOK-TA---	-----T-E	HCYAVHLLKE	-CATNBHORA	CHMLKILIN
	CKK_h	HATBO--KA	H--PPRBOCQ	PITTLCEAF	CKVFLAKAGE	LRE-CF---	-----A-E	TLVAVSLO-	-CKEDDEBOL	FMELHNFCK
	MEY_h	AYOVHYFOPB	SLJ--TH	FMKVIKDFM	CKVYHSTLLO	N-D-EK---	-----K	ILCAVHLLMR	-ITDISEYGO	FLCEJINAKO
	TAK_h	FEQACVHHIK	-----RMO3V	LKVELCEAF	CKVFLAECMH	LAP-EO---	-----D-K	ILVAVHLLK	-EABEBAAD	FOGPAZELTH
	AKL_h	TKKL--A	DVNVORHKA	LKTLCEAF	CKVYHCEGLO	N-D-SI---	-----C	ILVAVHLLK	-ATYABHLEO	FLJHATCHKE
	TIE_h	-P-EPL--S	YPMLEWEDIT	FEOLCEAF	CKVYHATIKK	D-GLK---	-----C	ILVAVHLLK	-YASBEMMO	PAGELELCK
	EPK_h	WTFPS--K	E--LDPANLH	NOTVCEAF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-TSFEGGVMH	PLNATINDO
	RYK_h	-KSKV--K	DEAJBEMJIT	LKVLCEAF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-GASEIOYTH	NLTICKLQ
	DOR_h	GDR--PRY	D--PPRSLR	PKKLCEDF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-GATEKMANO	FLKVKIMBR
	ADL_h	E--ZIE--H	LPAPPELDT	LMLCEAF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-GASTOGECE	FLKVKIMBR
	RET_h	TL-ED-PCW	E--PPKINLV	LEKTLCEAF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-GASTOGECE	FLKVKIMBR
	CTK_h	-P-CP-PGY	E--VSPANYT	LKALCEAF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-GASTOGECE	FLKVKIMBR
	ROR_h	KPKSL--K	E--LPLKAVT	PKSELCEAF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-GASTOGECE	FLKVKIMBR
	MUSK_h	MAKLE--L	E--YPMWIE	TYKOLCEAF	CKVYHCEGLO	EKO-PM---	-----C	ILVAVHLLK	-GASTOGECE	FLKVKIMBR
539	FFPR1_h	LGAKHKN3ML	LGACTG--CP	L-----TVIV	KINASE	YLD--HMPFG	LEVYHPSH-	-----NR--E-	EDL--SROL	
	EGFR_h	VON--PNUVRL	LGCTCTE--TV	D-----L-T	OLAPPGCLD	YVR--CHK-ON	-----BA	BNH--	PG--	-----H-
	INSR_h	FTC--HNVVRL	LGUVYKE--CP	T-----LVYM	OLMANECAL	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	POBPR_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	KDR_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	CKK_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	MEY_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	TAK_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	AKL_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	TIE_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	EPK_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	RYK_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	DOR_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	ADL_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	RET_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	CTK_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	ROR_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
	MUSK_h	LGPHLNIYVL	LGACTG--CP	I-----F-IIT	KYCFYGLUN	YLM--GLMP	-----F--L--SH	-----HPE(87)	-----KTK(55)	-----KPL--LEHL
601	FFPR1_h	VSCATOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	EGFR_h	LMNVDOVARG	KMYLEDSKIV	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	INSR_h	LSMGAELABO	KAYLNAKKEV	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	POBPR_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	KDR_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	CKK_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	MEY_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	TAK_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	AKL_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	TIE_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	EPK_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	RYK_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	DOR_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	ADL_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	RET_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	CTK_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	ROR_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
	MUSK_h	LSFTYOVARG	MEFLASKEIC	-----VTEH	VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH	-----VTEH
684	FFPR1_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	EGFR_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	INSR_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	POBPR_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	KDR_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	CKK_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	MEY_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	TAK_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	AKL_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	TIE_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	EPK_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	RYK_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	DOR_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	ADL_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	RET_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	CTK_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	ROR_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW
	MUSK_h	WSECV-LLWE	IFTLG--SPY	P--GUPFEE--	-----LF-ELL	KEOENHOKPB	NETMELTHNN	ROG--HAYPSO	RPTFKOLVED	LORVYALTSW

FIGURE 6A



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465  
 FGFR1\_h LPEDPRWELP RORLYLGG-P LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 SRC\_h GLAKDAVEIP RE&LRLEV-K LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 BRK\_h LPHWDWERP RE&FTLCR-K LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 BTK\_h GLGYQSWED PKOLTFK-E LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 CSK\_h EFRYSCWALN HKELKLD-T LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 ABL\_h SPNYDKWEME RTDITMKH-K LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 ZAP70\_h LKOKKLF-LK ROKLLIADIE LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 FES\_h AVPKDKWYLN MEDLYLGG-O LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 FAK\_h MPSTROYEIO RERIELGRC-O LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 JAK1\_h PTEVDPTHPE KRPLKRIR-O LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...  
 ACK\_h PLQSLTCLIG BKOLRLLE-K LK... LK... LK... LK... LK... LK... LK... LK... LK... LK...

543  
 FGFR1\_h NIMLGAET -DDSP-LYVI VEYASKOHLR EYLQARRPPG LETCYNPSHN PECOLSSKDL VGCAYGYARG NEYLASKCCI  
 SRC\_h KLYDLAYVVS -E-EP-IYIV TEYHKBGELL OPLKCE... SKYLRLPOL VDMAAQIABG HAYVERHHYY  
 BRK\_h HILALYAVVS YG-OP-VYII TELHAKGBLL ELLROSO... EKYLPLYSEL LDIANDVAEG MCYLESDNYI  
 BTK\_h KLYOLYGYCT KOR-P-IFII TEYHANGELL KYLR&H... RHRFQDOL LEMCKOVCEA MEYLESQFL  
 CSK\_h NLVOLLEGVIV EEKGG-LYIV TEYHAKGBLL OYLRR&... RSVLGQDOL LKPSLDYCEA MEYLECHNFV  
 ABL\_h NLVOLLEGVIV REP-P-FYII TEYHANGELL OYLRR&... ROEYMAVYL LYHATDSSA MEYLEKKNFV  
 ZAP70\_h YIVRLIGVCT AEA---LMLV MENACGGPLH KFLYSE... REEIPYSNV AELLHDSYMG MEYLEKKNFV  
 FES\_h YIVRLIGVCT -OKOP-IYIV MELVGGGDFL TFLNTE... CARLRVKT LQHYGDAIAQ MEYLEKCCI  
 FAK\_h HLYKLIQVIT ENP---VYII MELCYLGLER SFLQVR... KYSLDCLAL ILTAYOLSTA LAYLESKRFV  
 JAK1\_h NLYKYXGICT EDGCGNIGLI NEFLPSGSLK EYLPKN... KKKIKLKOO LKYAYOICKG NDYLESROYV  
 ACK\_h NLIRLYGVIV TPP---KKNV TELAPLGSL DRLRKH... GGHFLGLTL SRYAYOVLEG MCYLESKRFI

621  
 FGFR1\_h HQRLAARL VTEONVHKIA DFGARLIRK HIOYKXTYN GRLPVKNMFP AL-CORIYT HQSDVWSFGV LLWEIFTGCG  
 SRC\_h HQRLAARL YGENLYCKYA DFGARLIRK DNEYTAROGA -KFPJKWTAP GVALYGR-FT IKEDVWSFGI LLTELTGR  
 BRK\_h HQRLAARL YGENTLCKV DFGARLIRK EDYTL&H -NIPYKWTAP ALGRGH-YG TKEDVWSFGI LLHMFSGCO  
 BTK\_h HQRLAARL YHDOGVYKYS DFGARYVL DGEYTSVGS -YFPVWSPF EYLYBK-FS SKEDVWSFGI LHWEIYSLGK  
 CSK\_h HQRLAARL YSEDNYAKYS DFGARYVL -EASSTQDTG -XLPYKWTAP EALREKK-FS TKEDVWSFGI LLWEIYSFGR  
 ABL\_h HQRLAARL YGENMLYKVA DFGARYVL GOTYTAMAGA -KFPJKWTAP EBLAYNK-FS IKEDVWSFGI LLWEIATYGH  
 ZAP70\_h HQRLAARL LYNRHTAKIS DFGARKALQA DDYTTAKSA GKUPLKWTAP EDINFK-FS SRSDVWSYGC THWEALSYOO  
 FES\_h HQRLAARL YTEKMYLKIS DFGARYME DGYTAASGGG RDYVKEWTAP EALNYGR-YG STSDVWSFEL LLWETFSLGA  
 FAK\_h HQRLAARL VSSNOGVKLG DFGARYME DSTYTKA-SK CKLPKWNMFP SSIMFRR-FT SAEVWSFGV CMWEILMHGV  
 JAK1\_h HQRLAARL YESSHOVKIS DFGARYME DKEYTYKOD ROSPYFWYAP EELNOSK-FY JAEVWSFGV TLHLLTYCO  
 ACK\_h HQRLAARL LATROLVKIG DFGARYME DFGARYME NDDHYVROEM RKYPFAWCAP EELZTRT-FS HASVWSFGV TLWCHTYGO

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 FGFR1\_h S----- PTPGYP VEECLFKLKE -CHRNKPSK CTNELYMHNR DCHAYVPSOR PTFKDLVECL ORJVALTSNQ  
 SRC\_h Y----- PTPGNY NREVLDOVER -GYNMPPE CPESLMOLNC OCHKEPEER PTFEYLQAF LQYFTSTEPQ  
 BRK\_h Y----- PTPGHS NHEAPLRVDA -GYNMPPE CPESLMOLNC OCHKEPEER PTFEYLQAF LQYFTSTEPQ  
 BTK\_h Y----- PTERFT NSETAEHIAQ -GLRLYRPHL ASEKYTTINY SCHKEKADER PTFKTLLEN LQYFTSTEPQ  
 CSK\_h Y----- PTPRIP LKDVVPVVEK -CYKNOAPDG CPPAYVEYMK NCHLODAMR PTFKTLLEN LQYFTSTEPQ  
 ABL\_h S----- PTPGID LSQVYELLEK -DYNMERPEG CREKUYELMR ACHOWNPSOR PTFKTLLEN LQYFTSTEPQ  
 ZAP70\_h K----- PTKKMK QPEVMAFIE -QKKRMECPPE CPPELYALMS DCHYKWEOR PTFKTLLEN LQYFTSTEPQ  
 FES\_h S----- PTPNLB NQOTREFVEK -QKKRMECPPE CPPELYALMS DCHYKWEOR PTFKTLLEN LQYFTSTEPQ  
 FAK\_h K----- PFGQVK NNOYIGRIE -NGERLPHPPK CPPELYALMS DCHYKWEOR PTFKTLLEN LQYFTSTEPQ  
 JAK1\_h SSSPMALFL KNIGPTHQDM TYTRLYNTLK EDKRLPCPPH CPPELYALMS DCHYKWEOR PTFKTLLEN LQYFTSTEPQ  
 ACK\_h E----- PWIGLN GSQTLHKIQK EGERLPRPEO CPPELYALMS DCHYKWEOR PTFKTLLEN LQYFTSTEPQ

FIGURE 6B





## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification <sup>6</sup> : C12N 15/54, C07K 14/71, 14/705, C12N 9/12, 15/12, C12Q 1/48, G01N 33/68, C07D 209/34, A61K 31/40		A3	(11) International Publication Number: <b>WO 98/07835</b>
			(43) International Publication Date: 26 February 1998 (26.02.98)
(21) International Application Number: PCT/US97/14885		R. [US/US]; 5465 Sylvan Avenue, Riverdale, NY 10471 (US). McMAHON, Gerald [US/US]; 1800 Schultz Road, Kenwood, CA 95452 (US). TANG, Peng, C. [US/US]; 827 Camino Ricardo, Moraga, CA 94556 (US).	
(22) International Filing Date: 21 August 1997 (21.08.97)			
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(60) Parent Application or Grant (63) Related by Continuation US Not furnished (CIP) Filed on Not furnished			
(71) Applicant (for all designated States except US): SUGEN, INC. [US/US]; 351 Galveston Drive, Redwood City, CA 94063 (US).			
(72) Inventors; and (75) Inventors/Applicants (for US only): MOHAMMADI, Moosa [IR/US]; 564 First Avenue #12F, New York, NY 10016 (US). LI, Sun [CN/US]; 64 Rockharbor Lane, Foster City, CA 94404 (US). LIANG, Congxin [CN/US]; 726 W. Remington Drive, Sunnyvale, CA 94087-2242 (US). SCHLESSINGER, Joseph [IL/US]; 37 Washington Square West, New York, NY 10011 (US). HUBBARD, Stevan,		(74) Agents: WARBURG, Richard, J. et al.; Lyon & Lyon LLP, First Interstate World Center, Suite 4700, 633 West Fifth Street, Los Angeles, CA 90071-2066 (US).	
		(81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, ARIPO patent (GH, KE, LS, MW, SD, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).	
		Published With international search report.	
		(88) Date of publication of the international search report: 1 October 1998 (01.10.98)	
(54) Title: CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE			
(57) Abstract			
<p>The present invention relates to the three-dimensional structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates that define the structures of the protein tyrosine kinase and any of the compounds bound to it are pertinent to methods for determining the three-dimensional structures of protein tyrosine kinases with unknown structure and to methods that identify modulators of protein tyrosine kinase functions.</p>			

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## INTERNATIONAL SEARCH REPORT

International Application No  
PCT/US 97/14885

## A. CLASSIFICATION OF SUBJECT MATTER

IPC 6 C12N15/54 C07K14/71 C07K14/705 C12N9/12 C12N15/12  
C12Q1/48 G01N33/68 C07D209/34 A61K31/40

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 6 C07K C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	S. R. HUBBARD ET AL: "Crystal structure of the Tyrosine kinase domain of the human insulin receptor" NATURE., vol. 372, 22 December 1994, LONDON GB, pages 746-754, XP002061072 cited in the application see the whole document ---	1,2,6, 24,25,30
X	LEI WEI ET AL: "Expression, characterization, and crystallization of the catalytic core of the human insulin receptor protein-tyrosine kinase domain" JOURNAL OF BIOLOGICAL CHEMISTRY., vol. 270, no. 14, 1995, MD US, pages 8122-8130, XP002061073 see page 8129, last paragraph - page 8130 --- -/--	1,2,24, 25,30

☒ Further documents are listed in the continuation of box C.☒ Patent family members are listed in annex.

## \* Special categories of cited documents:

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Date of the actual completion of the international search

17 April 1998

Date of mailing of the international search report

27.07.1998

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LE CORNEC N.D.R.

# INTERNATIONAL SEARCH REPORT

Patent Application No

PCT/US 97/14885

## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
------------	--	-----------------------

8

A

WO 92 13870 A (THE REGENTS OF THE  
UNIVERSITY OF CALIFORNIA) 20 August 1992  
see claims 26-28

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24,25,27

2

# INTERNATIONAL SEARCH REPORT

International application No.

PCT/US 97/ 14885

## Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:  
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☐ Claims Nos.:  
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
3. ☐ Claims Nos.:  
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

## Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see annex

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

subject 1 (Please see Extra sheet)

### Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

## FURTHER INFORMATION CONTINUED FROM PCT/ISA/

1. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: PDGF-R. The polypeptide and the method used to form the crystal.

2. Claims: 1-3, 6, 24-25, 27, 30 all partially .

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase:FLK/KDR. The polypeptide and the method used to form the crystal.

3. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: CCK4. The polypeptide and the method used to form the crystal.

4. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: MET. The polypeptide and the method used to form the crystal.

5. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: TRKA. The polypeptide and the method used to form the crystal.

6. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: AXL. The polypeptide and the method used to form the crystal.

7. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: TIE. The polypeptide and the method used to form the crystal.



## FURTHER INFORMATION CONTINUED FROM PCT/ISA/

8. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: EPH. The polypeptide and the method used to form the crystal.

9. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: RYK. The polypeptide and the method used to form the crystal.

10. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: DDR. The polypeptide and the method used to form the crystal.

11. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: ROS. The polypeptide and the method used to form the crystal.

12. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase receptor: RET. The polypeptide and the method used to form the crystal.

13. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: LTK. The polypeptide and the method used to form the crystal.

14. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: ROR1. The polypeptide and the method used to form the crystal.

15. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: MUSK. The polypeptide and the method used to form the crystal.

## FURTHER INFORMATION CONTINUED FROM PCT/ISA/

16. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: SRC. The polypeptide and the method used to form the crystal.

17. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: BRK. The polypeptide and the method used to form the crystal.

18. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: BTK. The polypeptide and the method used to form the crystal.

19. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: CSK. The polypeptide and the method used to form the crystal.

20. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: ABL. The polypeptide and the method used to form the crystal.

21. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: ZAP70. The polypeptide and the method used to form the crystal.

22. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: FES. The polypeptide and the method used to form the crystal.

## FURTHER INFORMATION CONTINUED FROM PCT/ISA/

23. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: FAK. The polypeptide and the method used to form the crystal.

24. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: JAK. The polypeptide and the method used to form the crystal.

25. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: ACK. The polypeptide and the method used to form the crystal.

26. Claims: 1, 24-25, 27, 30 all partially and 7-23, 29, 31-34 all completely.

Crystalline form of a polypeptide corresponding to the catalytic domain of a FGF receptor protein tyrosine kinase which is complexed or not with a compound. The polypeptide (cDNA encoding it) and the method used to form the crystal. The cDNA encoding FGFR tyrosine kinase as in seq ID. no 5.

27. Claims: 35-42 completely

Method to determine the three dimensional structure of receptor and/or non-receptor tyrosine kinases.

28. Claims: 43-50

Method of identifying a potential modulator of protein tyrosine kinase function by using a three dimensional computer representation.

29. Claims: 51-54, 57 all completely and 58-61 all partially

A modulator of protein tyrosine kinase function and its use in a method of treating a disease.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/

30. Claims: 55 completely and 58-61 all partially

Method of identifying a potential modulator of protein tyrosine kinase by comparing the level of protein kinase phosphorylation between cells not administered the potential modulator and cells administered said potential modulator.

31. Claims: 56 completely and 58-61 all partially

Method of identifying a potential modulator of protein tyrosine kinase by comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator.

# INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/US 97/14885

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 9213870 A	20-08-1992	AU 669328 B	06-06-1996
		AU 1346792 A	07-09-1992
		CA 2101632 A	01-08-1992
		EP 0572505 A	08-12-1993
		EP 0811685 A	10-12-1997
		EP 0811686 A	10-12-1997
		JP 6505629 T	30-06-1994
		NZ 241479 A	27-09-1994
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